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THE CONTROL OF OXIDES OF NITROGEN EMISSIONS FROM AIRCRAFT GAS TURBINE ENGINES

Volume 2: The NOx Formation Process

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16. Abstract

The objective of this study was to develop criteria for use in the design of aircraft gas turbine combustion chambers to minimize nitrogen oxide emissions. The approach adopted involved the development of a mathematical model of NOx emission from aircraft engine combustors; a parametric analysis, using the model, to determine the sensitivity of NOx emissions to variations of model parameters and engine design variables; evaluation of critical model parameters by means of experimental measurements; and the incorporation of the model into combustor design methods to provide guidelines for minimizing NOx emission while maintaining other performance and emission characteristics. The results of the study and the NOx emission control criteria are described in Volume 1 (FAA-RD-71-111-1). Volume 2 (FAA-RD-71-111-2) describes the nitric oxide formation process and a computer program (NOXRAT) for calculating thermodynamic data. The program is based upon a six-reaction model of NO formation. Volume 3 (FAA-RD-71-111-3) describes combustion and flow processes in gas turbine combustors and a computer program (GASNOX) for calculating gas properties and NO concentrations throughout a combustor. This program is based upon a three-zone, heterogeneous model of gas turbine combustor operation. Program GASNOX is used with input data from Program NOXRAT to calculate NO emission rates.

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1. INTRODUCTION

Volume 1 of this report carries a full description of the complete program but omits mathematical details of the model developed to predict the nitric oxide (NOx) emissions from aircraft gas turbine combustors and also the details of two computer programs developed as part of the study for obtaining predictions from the model. It is the purpose of Volumes 2 and 3 of the report to present full descriptions of both the model and the computer programs.

It is convenient to consider the model in two parts, one part being concerned with the NOx formation process and the other with modeling the flow behavior within gas turbine combustors. The convenience arises not only due to the basic difference in the studies of these two parts, but also due to the fact that a separate computer program has been developed for each part. This approach has been adopted in the interests of economy of computation as calculation of the necessary data for the determination of the NOx formation process requires appreciable computer time, but, of course, the data once collected can be applied to any combustor calculation with the same reference conditions (in this case, combustor inlet conditions) of pressure and temperature. The computer program developed for this task has the name NOXRAT, and its function is to compute the rate terms of the NOx formation process and all relevant thermodynamic data for a series of fuel-to-air ratios with a common reference state.

Volume 2 of this report is solely concerned with the nitric oxide formation process. It presents a mathematical description of the process, a full description of the program NOXRAT, and also includes a section which is essentially a user's manual for the program. Volume 3 produces the same details for the flow model developed to describe the flow conditions in a gas turbine combustor. The corresponding computer program is named GASNOX and it is so arranged that the rate terms and all relevant thermodynamic data computed in NOXRAT are punched onto a deck of computer cards which serves as input data to the main program GASNOX.

The objective of this volume of the report, therefore, is to present the theory behind the NOx formation process and details of the computer program developed for its application.

2. THE NOx FORMATION PROCESS

While engine exhaust emissions are often expressed as nitrogen oxides (NOx), or as nitrogen dioxide (NO_2), the pollutant present in the exhaust gas as it leaves the engine is almost completely nitric oxide, NO, with only a few per cent of NO_2 (Ref 1). The conversion to NOx or NO_2 is made because many of the techniques used to measure nitric oxide require first that it be oxidized to nitrogen dioxide. Thus, inside the engine, the important oxide of nitrogen to consider is nitric oxide, NO.

Several authors have proposed reaction schemes for nitric oxide formation, e.g., Caretto, Sawyer, and Starkman (Ref 1), Bartok, et al (Ref 2), Newhall (Ref 3), Lavoie, Heywood, and Keck (Ref 4). The set of reactions proposed by Lavoie, et al (Ref 4) is the most complete for predicting nitric oxide formation, and it has been evaluated experimentally for a range of equivalence ratios (0.9-1.2), pressures (10-30 atm), and temperatures (2200-2800 deg K) in a spark-ignition engine (Refs 4 and 5). These conditions are directly comparable to those occurring in the gas turbine combustor primary zone as shown by Heywood et al (Ref 6), and the reaction scheme does predict NO emission levels which are in good agreement with measurements made on such combustion systems.

The set of reactions included in the analyses of References 4, 5, and 6 are incorporated in the model and are shown below.

$$N+NO \rightleftharpoons N_2+O \quad (1)$$
$$N+O_2 \rightleftharpoons NO+O \quad (2)$$
$$N+OH \rightleftharpoons NO+H \quad (3)$$
$$H+N_2O \rightleftharpoons N_2+OH \quad (4)$$
$$O+N_2O \rightleftharpoons N_2+O_2 \quad (5)$$
$$O+N_2O \rightleftharpoons NO+NO \quad (6)$$

Note that the reaction $2NO \rightleftharpoons N_2+O_2$ has been omitted from this scheme as it is very slow and does not proceed directly. In References 4 through 6 the rate constants selected for these reactions were taken from Schofield (Ref 7) except for reaction 3 which was taken from

Campbell and Thrush (Ref 8). These constants are,

$$k_1 = 2 \times 10^{-11}$$
$$k_2 = 2 \times 10^{-11} \exp(-7.1/RT)$$
$$k_3 = 7 \times 10^{-11}$$
$$k_4 = 5 \times 10^{-11} \exp(-10.8/RT)$$
$$k_5 = 6 \times 10^{-11} \exp(-24.0/RT)$$
$$k_6 = 8 \times 10^{-11} \exp(-24.0/RT)$$

and are in cm^3/sec-molecule. R is in kcal/gm-mole-deg K. Since the equilibrium constants for these reactions are known, the kinetic scheme is thus completely defined.

Recently completed analyses of data and correlations available in the latest literature have raised some question as to the reliability of the above constants. A group at Leeds University (Ref 9) reports k_1 better correlated in the form Aexp(-E/RT) while both Leeds and Newhall (Ref 3) show reaction 2 to be correlated more satisfactorily in the form AT exp(-E/RT). Newhall also correlated reaction 6 with a pre-exponential factor 3.6 times greater, and an activation energy 1.16 times greater, than the corresponding values determined by Schofield.

With this lack of agreement of the rate constants, it was decided to represent all six reactions in the reaction scheme in the general form,

$$k_i = A_i T_i^{n} \exp(-E_i/RT) \tag{7}$$

This format allows maximum flexibility in comparing the different fits of the kinetic rate data for each of the expressions. Further, as new data and correlations become available, it will be a simple matter to adjust the three constants to correspond accordingly to those correlations and data.

Not all of the above reactions are equally important over the equivalence ratio and temperature range of interest. The first two reactions, the Zeldovich chain mechanism, are the two most important reactions at high temperatures (greater than 2200 deg K) in fuel-lean mixtures. The importance of this pair of reactions is well established. The third reaction becomes important in fuel-rich mixtures. Reactions

4, 5, and 6 involving N_2O as an intermediary become important at temperatures about 2000 deg K. It can be shown that the small amount of NO_2 present is in equilibrium with the NO and other reactions with NO_2 need not be included (Ref 5).

Conditions in gas turbine combustors fall into all of these regimes, but calculations indicate that the reactions 4, 5, and 6 do not contribute greatly to the nitric oxide formation rate. In fact, if one accepts the probable limits of accuracy for any such kinetic scheme, a case may be made for their exclusion. However, these reactions are included in the reaction scheme for the sake of completeness.

In order to apply this reaction scheme to gas turbine combustors, it is necessary to be able to predict the concentration levels of all species active in the set of six reactions specified above at all thermodynamic states typical of the combustor. At the pressure and temperature levels that exist in such combustors during high thrust, low altitude operation, the hydrocarbon oxidation reactions go rapidly to completion compared with the nitric oxide formation processes. In order to predict these specie concentrations therefore, the following assumptions are made:

a. Combustion is mixing controlled and not rate-limited, and therefore, in the combustor, N_2, O_2, O, OH, H, and H_2 concentrations are the equilibrium concentrations corresponding to the combustor inlet temperature and pressure, and to the equivalence ratio. This assumption limits the usefulness of the model to high pressure, high temperature operating conditions, but it is precisely these conditions at which most nitric oxide is produced and are therefore of most interest to this study.

b. N and N_2O concentrations are given by the steady-state assumption; That these concentrations are not in equilibrium but are in steady-state with NO can be shown by deriving rate equations for N and N_2O which have relaxation times short compared with the NO rate equation.

If these assumptions are applied to Equations 1 through 7, then the change, $\dot{r}$, in total nitric oxide per unit time per unit volume,

that results from chem cal reaction over a fixed element can be written as

$$\dot{r} = 2M_{NO}(1-\alpha^2)\left[\frac{R_1}{1+\alpha K_1}+\frac{R_6}{1+K_2}\right] \quad (8)$$

where M_{NO} is the molecular weight of NO, $\alpha = [NO]/[NO]_e$ is the local nitric oxide concentration divided by the equilibrium nitric oxide concentration, R_1 is the "one-way" equilibrium rate of reaction 1, i.e., $R_1 = k_1 \; [N]_e \; [NO]_e$; $K_1 = R_1/(R_2+R_3)$ with R_2 and R_3 defined analogously to R_1 but for reactions 2 and 3; and $R_6 = k_6 \, [O]_e \, [N_2O]_e$ and $K_2 = R_6/(R_4+R_5)$.

It is interesting to consider the form of the equation above when applied to the gas turbine combustor. In this case the thermodynamic base state is represented by the combustor inlet pressure and temperature, both of which are nonvariable with time for a fixed operating condition. If the fuel-to-air ratio is specified, therefore, the terms R_1, R_6, K_1 and K_2 all become constants as a consequence of assumptions a and b above. The molecular weight M_{NO} is a constant, hence the only variable is α and the equation reduces to the simple form,

$$dNO/dt = f(NO)$$

which may readily be integrated to follow the nitric oxide concentration levels through the combustor.

Maximum utility has been made of this simplicity, chiefly in the interests of reducing the computer operating costs for each sample case tested in the flow model. The computational procedure, as previously explained in the introduction, was separated into two tasks; the first task primarily determines the rate terms R_1, R_6, K_1, and K_2 for a specified combustor inlet temperature and pressure over the complete range of fuel-to-air ratios that cause sufficiently high temperatures to form nitric oxide, and the second task computes the flow conditions throughout the combustor and uses the data collected from task one to predict nitric oxide emission levels.

A computer program has been developed for each task and the program for Task 1 will be described in the next section.

3. PROGRAM NOXRAT

3.1 INTRODUCTION

3.1.1 Program Function and Capabilities

Program NOXRAT is a modified version of CEC, a NASA developed digital computer program written in Fortran IV (Refs 10, 11 and 12). NOXRAT is designed to evaluate the chemical equilibrium products, the adiabatic flame temperature, and the kinetic properties used in the nitric oxide formation model (previously described) for the combustion of a reactive fuel, or a fuel mixture with an oxidant or mixture of oxidants. NOXRAT iteratively calculates the equilibrium properties of the combustion products based on a minimized Gibbs free energy. In a typical equilibrium computation NOXRAT prints the following properties for each assigned fuel-to-air ratio:

a. The equilibrium temperature and pressure; the sonic velocity, the enthalpy, entropy, mean molecular weight, $(\partial V/\partial P)_T$, the heat capacity, and the heat capacity ratio (C_p/C_v), of the combustion stream.*

b. The mole fraction of each of the combustion products present at equilibrium at concentrations greater than 5×10^{-6}.*

c. The chemical formula, weight fraction in the total fuel or oxidant, and the base enthalpy, temperature, density, and physical state of each of the specified reactants.*

d. The total oxidant to total fuel weight ratio, the per cent fuel, the equivalence ratio, and the average density of the reaction mixture.*

e. The equilibrium mole fraction of each of the species of interest in the nitric oxide kinetic scheme (Ref 18) and the equilibrium mole fractions of $C_{(s)}$, CO, and CO_2.

f. The molecular weight and the adiabatic flame temperature of the combustion products; the assigned inlet pressure; the

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*Normal output of CEC.

fuel-to-air ratio; and the atomic composition, inlet temperature, and enthalpy of both the fuel(s) and the oxidant(s).

For each assigned pressure the program also prints and punches:

a. The atomic composition of the fuel (C_xH_y); the inlet air temperature; a code number identifying the set of kinetic constants used in the NO rate formation calculations; the assigned pressure; and the stoichiometric equivalence ratio.

b. For each specified fuel-to-air ratio: the mixture ratio (mass of fuel to mass of fuel and air); the equivalence ratio; the density and adiabatic flame temperature of the combustion products; the equilibrium concentration of NO, CO, $C_{(s)}$, and CH_2 (unburned fuel); and the kinetic parameters* R_1, R_6, K_1, and K_2 where R_1 and R_6 are forward reaction rates for reactions 1 and 6 and K_1 and K_2 are ratios of forward reaction rates used in the kinetic scheme (see Appendix V).

NOXRAT also permits calculation of:

a. Chemical equilibrium for assigned temperatures and pressures.

b. Theoretical rocket performances for both frozen and equilibrium compositions during expansion.

c. Chapman-Jouguet detonation properties.

The latter two options were not exercised in this study.

3.1.2 Analysis Procedures

The analytical procedures on which NOXRAT is based are described in Section 2. A detailed description of the changes that have been incorporated into these procedures to permit calculation of the reaction rate constants and the thermal properties used in the chemical

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* These parameters are used to compute the rate of change of the NO mass fraction due to chemical reaction by:

$$d\{NO\}/dt = \frac{2M_{NO}}{\rho}(1-\alpha^2)\left[\frac{R_1}{1+\alpha K_1} + \frac{R_6}{1+K_2}\right]$$

where M_{NO} is the molecular weight of NO, ρ is the gas density, $\{NO\}$ is the mass fraction concentration of NO and α is the ratio of NO concentration to the NO concentration at equilibrium.

reaction scheme for the formation of nitric oxide are presented in the appendices of this report. Reference to any of these procedures is unnecessary for operation of the computer program.

3.1.3 Report Arrangement

The main body of the report begins with a section in which the input data necessary for the solution of any case are described in detail; this includes instructions for preparing and supplying these data to the program and a sample case in the appropriate format. The next section contains a discussion of the various types of output data which are obtained from the program and also the output data from the sample case. Following that is a section containing miscellaneous information regarding the operation of the program with the CDC 6600 computing system. The next section is a description of the error messages printed by the program.

The first appendix consists of a general discussion of the overall logic structure of the program. The next appendix gives the Fortran nomenclature for the major new variables incorporated into the original CEC program. The remaining appendices, except the last two, provide detailed description of the changes made to existing routines and of the subroutines which have been developed and incorporated into the program, one appendix for each routine. The appendix for each new subroutine contains a presentation of the input and output variables, an internal Fortran nomenclature, a description of the step-by-step calculation procedure, and a Fortran listing of the subroutine. The last two appendices are respectively a listing of the program in its entirety and a listing of the THERMO data.

3.2 INPUT DATA

3.2.1 General Description

The input data to Program NOXRAT is nearly identical with that of NASA's Program CEC. Although the input format for CEC has been described in a preliminary guide (Ref 13) and detailed in a NASA report (Ref 14), NREC has elected to present here

a description of NOXRAT input (and output) data. This description is suitable to allow the reader to understand the mechanics of how to operate the program. Much of this information is taken directly from Reference 13.

Program input data will be discussed under four categories. Three of the categories are required and one is optional. The three required categories and the code names by which they will be referred are as follows:

a. Library of thermodynamic data for reaction products (THERMO data).

b. Data pertaining to reactants (REACTANTS cards).

c. Namelist data which includes the type of problem, required schedules, and options (NAMELISTS Input).

d. The optional category of data are chemical formulas of species which are singled out for special purposes (OMIT and INSERT cards).

THERMO Data

The thermodynamic data are in the form of 7 least squares coefficients (a_i) for the following equations:

$$\frac{C_P^\circ}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \tag{1}$$

$$\frac{H_T^\circ}{RT} = a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + \frac{a_6}{T} \tag{2}$$

$$\frac{S_T^\circ}{RT} = a_1 \ln T + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 + \frac{a_5}{4} T^4 + a_7 \tag{3}$$

$$\frac{G_T^\circ}{RT} = \frac{H_T^\circ}{RT} - \frac{S_T^\circ}{R} \tag{4}$$

For each species, two sets of coefficients are included for two adjacent temperature intervals. The data provided cover the temperature intervals 300 deg K to 1000 deg K and 1000 deg K to 5000 deg K.

The supplied data for each species were made by the PAC program described in NASA TN D-4097 (Ref 15). For the gases, the PAC program calculated the thermodynamic functions from the molecular data given in JANAF (Ref 16). For the condensed species, the thermodynamic functions were taken directly from JANAF. However, NASA added the functions at the transition points since they were not included in the JANAF data. The PAC program does a least squares fit of the functions for the two specified temperature intervals. The fits are constrained to give consistent data at transition points and at the common interval temperature (1000 deg K).

Heats of formation and transition were also taken from JANAF. They were combined with sensible heats to give assigned enthalpies H_T^o. By definition,

$$H_T^o \equiv H_{298.15}^o + \left[H_T^o - H_{298.15}^o\right] \tag{5}$$

It has been arbitrarily assumed that $H^o_{298.15} = (\Delta H^o_f)_{298.15}$. Equation 5 then becomes

$$H_T^o \equiv (\Delta H_f^o)_{298.15} + \left[H_T^o - H_{298.15}^o\right] \tag{6}$$

For the JANAF reference elements, $H^o_{298.15} = 0$. In general, $H^o_T \neq (\Delta H^o_f)_T$ for $T \neq 298.15^o K$.

REACTANTS Data

Reactants data consists of the following physical data for each of the reaction species in the combustion stream.

a. Atomic symbols and formula numbers.
b. Relative weights or number of moles (for fuel in total fuels or oxidant in total oxidants).
c. Enthalpy.
d. Physical state (solid, liquid, gas).
e. Temperature associated with enthalpy in item c above.
f. Density.

NAMELISTS Data

NAMELISTS data is specified on two input NAMELISTS; only the first is necessary for generation of the chemical equilibrium and kinetic rate data of interest. The second NAMELIST is associated with the rocket performance option of NOXRAT described in the introduction to this report. This latter option was not exercised in this study but will be described in the following subsection. The information required in the first NAMELIST is:

a. The type of problem.

b. One or more pressures.

c. One or more temperatures for assigned temperature problems (e.g., rocket problems with an assigned chamber temperature).

d. The relative amount of fuel(s) and oxidant(s).

The information required in the second NAMELIST is:

a. The pressure ratio schedule.

b. The subsonic area ratio values (optional).

c. The supersonic area ratio values (optional).

d. Whether only frozen or equilibrium performance is to be calculated (optional).

OMIT and INSERT Data

OMIT and INSERT cards are optional. They contain the names of particular species in the library of thermodynamic data for the specific purposes stated below.

OMIT Cards. These cards list species to be omitted from the THERMO data.

INSERT Cards. These cards contain the names of condensed species only.

3.2.2 Detailed Description of Input Data

The information required to prepare the input data for a case is furnished in the table given below. This information contains a description of each input item as well as a description of the form in

which these items are written on input data sheets. The descriptions of the input items refer frequently to several points, relevant to the selection of input values, which are discussed in the subsequent subsection. The discussions of these points provide additional detailed information useful in preparing the input data for any case.

The first input item read by Program NOXRAT is the code word THERMO. The second input line contains the three temperature values 300, 1000, 5000. This input is followed by the thermodynamic data for any number of species. The last line of the THERMO input contains the code word END and follows the last set of species data (see point a).

Line	Location	Input Item	Type of Number	Fortran Symbol	Description
1	1-6		A		This is the code word "THERMO" that identifies the beginning of the thermodynamic data
2	1-10		FP	TLOW	Low temperature for lowest temperature interval of thermodynamic data
2	11-20		FP	TMID	Common temperature for the two temperature intervals of the thermodynamic data
2	21-30		FP	THIGH	High temperature for highest temperature interval of thermodynamic data
3	1-12		A	DATA	Species name
3	19-24		A	DATA	Date
3	25-26		A	DATA	Atomic symbol
3	27-29		FP	DATA	Atomic formula number
3	30-31		A	DATA	Atomic symbol
3	32-34		FP	DATA	Atomic formula number

Line	Location	Input Item	Type of Number	Fortran Symbol	Description
3	35-36		A	DATA	Atomic symbol
3	37-39		FP	DATA	Atomic formula number
3	40-41		A	DATA	Atomic symbol
3	42-44		FP	DATA	Atomic formula number
3	45		A	DATA	Species phase (S = solid; L = liquid; G = gas)
3	46-55		FP	DATA	Low temperature of temperature interval
3	56-65		FP	DATA	High temperature of temperature interval
3	80		Int	NCD	Integer 1 to identify card
4	1-15	a_1	FP	DATA	Coefficient in equations 1-4 for upper temperature interval
4	16-30	a_2	FP	DATA	Coefficient in equations 1-4 for upper temperature interval
4	31-45	a_3	FP	DATA	Coefficient in equations 1-4 for upper temperature interval
4	46-60	a_4	FP	DATA	Coefficient in equations 1-4 for upper temperature interval
4	61-75	a_5	PP	DATA	Coefficient in equations 1-4 for upper temperature interval

Line	Location	Input Item	Type of Number	Fortran Symbol	Description
4	80		Int	NCD	Integer 2 to identify card
5	1-15	a_6	FP	DATA	Coefficient in equations 1-4 for upper temperature interval
5	16-30	a_7	FP	DATA	Coefficient in equations 1-4 for upper temperature interval
5	31-45	a_1	FP	DATA	Coefficient in equations 1-4 for lower temperature interval
5	46-60	a_2	FP	DATA	Coefficient in equations 1-4 for lower temperature interval
5	61-75	a_3	FP	DATA	Coefficient in equations 1-4 for lower temperature interval
5	80		Int	NCD	Integer 3 to identify card
6	1-15	a_4	FP	DATA	Coefficient in equations 1-4 for lower temperature interval
6	16-30	a_5	FP	DATA	Coefficient in equations 1-4 for lower temperature interval
6	31-45	a_6	FP	DATA	Coefficient in equations 1-4 for lower temperature interval

Line	Location	Input Item	Type of Number	Fortran Symbol	Description
6	46-60	a_7	FP	DATA	Coefficient in equations 1-4 for lower temperature interval
6	80		Int	NCD	Integer 4 to identify card

Lines 3-6 are repeated for each species in the thermodynamic data. The last line of the thermodynamic data, designated as line N below, contains the word END. This word is a signal to the computer that it has reached the end of the thermodynamic data.

N	1-3		A		This is the code word "END" that identifies the end of the thermodynamic data

The next set of input data read by Program NOXRAT are reactants cards (see point b) These cards are required for all problems; they contain specific data on the reactants to be combusted. The first item in the set contains the code word REACTANTS; the last card in the set is blank. In between the first and last cards may be any number of cards up to a maximum of 15, one for each reactant species being considered. There is no limit to the number of sets of reactants to be considered by the program; each must, however, be followed by appropriate data from input categories (3) and (4). The input for each series or set of reactants begins with a new data line N+1 and concludes with data line M.

Line	Location	Input Item	Type of Number	Fortran Symbol	Description
N+1	1-9		A		This is the code word "REACTANTS" that identifies the beginning of reactants data
N+2	1-2		A	NAME	Atomic symbol
N+2	3-9		FP	ANUM	Atomic formula number
N+2	10-11		A	NAME	Atomic symbol

Line	Location	Input Item	Type of Number	Fortran Symbol	Description
N+2	13-18		FP	ANUM	Atomic formula number
N+2	19-20		A	NAME	Atomic symbol
N+2	21-27		FP	ANUM	Atomic formula number
N+2	28-29		A	NAME	Atomic symbol
N+2	30-36		FP	ANUM	Atomic formula number
N+2	37-38		A	NAME	Atomic symbol
N+2	39-45		FP	ANUM	Atomic formula number
N+2	46-52		FP	PECWT	Relative weight (or number of moles) of fuel in total fuel or oxidant in total oxidant*
N+2	53		A	MOLE	Symbol to identify if PECWT is relative weight or number of moles = blank if relative weights = M if number of moles
N+2	54-62		FP	ENTH	Enthalpy in calories/gm mole (see point c)
N+2	63		A	FAZ	State = S for solid = L for liquid = G for gas
N+2	64-71		FP	RTEMP	Temperature in deg K associated with enthalpy in columns 54-62
N+2	72		A	FOX	Symbol to identify if reactant is an oxidant or a fuel = F if fuel = O if oxidant
N+2	73-80		FP	DENS	Density in gm/cc (optional)

---

* A fuel (or oxidant) may be composed of more than one fuel (or oxidant).

Line N+2 is repeated for each reactant in the set up to a maximum of 15 reactant species. The last line in this sequence (M) is blank.

M	1-80	Blank card

The next input items are read into Program NOXRAT using a NAMELIST statement. Input data referring to a NAMELIST statement begins with a $ in the second location on a new line, immediately followed by the NAMELIST name, immediately followed by one or more blank characters. Any combination of three types of data items may then follow. The data items must be separated by commas. If more than one line is needed for the input data, the last item on each line, except the last line, must be a number followed by a comma. The first location on each line should always be left blank since it is ignored. The end of a group of data is signaled by a $ immediately after the last item of data. The form that data items may take is:

a. Variable name = constant, where the variable name may be an array element or a simple variable name. Subscripts must be integer constants.

b. Array name = set of constants separated by commas where k* constant may be used to represent k consecutive values of a constant. The number of constants must be equal to the number of elements in the array.

c. Subscripted variable = set of constants separated by commas where, again, k* constant may be used to represent k consecutive values of a constant. This results in the set of constants being placed in consecutive array elements, starting with the element designated by the subscripted variable.

The first input NAMELIST is necessary for all of the options associated with Program NOXRAT. The items in this NAMELIST, INPT2 are:

Fortran Symbol	Input Item	Description
KASE		Optional assigned number associated with the case

Fortran Symbol	Input Item	Description
P	P	Assigned pressures (maximum of 26) Chamber pressure (one value) for rocket problems. Values in atm unless PSIA or MMHG are set TRUE (see below)
T	T	Assigned temperature in deg K (maximum of 26) (see point d)
MIX		Value of fuel-to-oxidant air weight ratios if FA is set TRUE (maximum of 40). For rocket problems (RKT is set TRUE) there must be as many sets of RKTINP NAMELIST inputs as there are MIX values (see point e)
FA		If variable is set TRUE, fuel-to-air weight ratios given in MIX. Value before read: FALSE
TP		If variable is set TRUE, problem type is assigned temperature and pressure Value before read: FALSE (see point f)
HP		If variable is set TRUE, problem type is assigned enthalpy and pressure. Value before read: FALSE (see point g)
RKT		If variable is set TRUE, problem type is rocket. Value before read: FALSE (see point h)
DETN		If variable is set TRUE, problem type is detonation. Value before read: FALSE (see point i)
PSIA	P	If set TRUE, pressure is in psia units Values are converted to atm internally Value before read: FALSE
MMHG	P	If set TRUE, pressure is in mmHg. Values are converted to atm internally. Value before read: FALSE
IONS		If set TRUE, ionic species are considered in the combustion products. Value before read: FALSE

Fortran Symbol	Input Item	Description
IDEBUG		If set TRUE, intermediate output is printed. Value before read: FALSE.

The second NAMELIST, RKTINP, is required only for rocket (RKT) problems. It follows the INPT2 namelist. The items in this NAMELIST are

PCP		Ratio of chamber pressure to exit pressure (maximum of 22 values). See point j.
EQL		If set FALSE, program will not calculate rocket performance assuming equilibrium composition during expansion. Value before read: TRUE. This is an optional input. See point k.
FROZ		If set FALSE, program will not calculate rocket performance assuming frozen composition during expansion. Value before read: TRUE. This is an optional input. See point k.
SUBAR		Subsonic area ratio. This is an optional input. See point l.
SUPAR		Supersonic area ratio. This is an optional input. See point l.

The remaining input items to Program NOXRAT are optional. These are OMIT and INSERT cards. Each card contains the word OMIT (in card columns 1 through 4) or INSERT (in card columns 1 through 6) and the names of from 1 to 4 species starting in columns 16, 31, 46, and 61. The names must be exactly the same as they appear in the THERMO data. See point m for further discussion of these input items.

3.2.3 Discussion of Input Data

Some important aspects to be considered in appropriately specifying the input data are discussed below. Reference to these discussions has been made in the preceding subsection in which the input format was described. The points referred to are as follows:

a. The library of thermodynamic data for reaction products may be read either from cards or from tape. If the data are read in from cards, the program will write these data on tape 4. During a computer run, the appropriate reaction product data for each new set of REACTANTS cards will be selected from tape 4 and stored.

THERMO data may be read in from cards for each run. However, a permanent tape or disc containing the data may be made during any run by using the required type of control cards preceding the operating deck. Two advantages of using a permanent tape or disc are that the scratch tape will not be made for each run and handling the cards is eliminated.

b. The fuel specification card(s) must preceed the oxidant card(s) in the input deck. Further, the oxygen must be the second specie specified in the oxidant air atomic formula; the atomic formula of the fuel must be specified in the order: carbon, hydrogen.

For gaseous mixtures (such as air) specify equivalent formula numbers on an atomic basis-- e.g., air is 78.03 per cent N_2, 20.99 per cent O_2, 0.98 per cent Ar. Air's equivalent formula is then $N_{0.7803}O_{0.2099}Ar_{0.0049}$ where the sum of the relative weights is as close to 1.0 as possible.

c. This enthalpy is not required for assigned temperature problems, i.e., TP.

d. If no T value is given the program uses the temperature and enthalpies on the reactant cards. When T values are assigned in the INPT2 NAMELIST, the program calculates the enthalpy from the library of THERMO data if the following two conditions are satisfied:

  i. The reactant card has zeros punched in card columns 37 and 38.

  ii. The reactant is a species in the library of THERMO data.

e. Relative amounts of fuel(s) and oxidizer(s). These quantities

may be specified by assigning 1 and 40 values for FA if no value is assigned for any of these, the program assumes the relative amounts of fuel(s) and oxidizer(s) to be those specified on the reactants cards.

f. TP Problem. Thermodynamic properties will be calculated for all combinations of assigned values for pressure P and temperature T in the NAMELIST. Thus, if 26T values and 26P values are included in the INPT2 lists, properties will be calculated for 676 P and T combinations.

g. HP Problem. Combustion temperature and corresponding properties will be calculated for each pressure specified.

h. RKT Problem. One pressure value P is required for the chamber pressure. The T schedule is used only if expansion from an assigned chamber temperature is desired (such as for a nuclear rocket). Otherwise it should be omitted.

The RKT problem requires a second namelist for input (RKTINP) discussed in the previous subsection.

i. DETN Problem. The temperature and pressures in the T and P input refer to the unburned gas.

j. The list of pressure ratios should <u>not</u> include values for the chamber and the throat. Values should be in increasing order.

k. The program will calculate both equilibrium and frozen performance unless RKTINP contains FROZ = F or EQL = F. If FROZ = F, only equilibrium performance will be calculated. If EQL = F, only frozen performance will be calculated.*

l. The subsonic area ratio values (SUBAR) and/or the supersonic area ratio values (SUPAR) are optional. When assigned area ratios are included, the PCP input should contain values of pressure ratios whose corresponding area ratios will be in the range of the assigned area ratios.

m. If OMIT cards are not used, the program will consider as possible species all those species in the THERMO data which are consistent with the chemical system being considered.

---

* F is the symbol for FALSE.

Occasionally, it may be desired to specifically omit one or more species from consideration as possible species. This may be accomplished by means of OMIT cards.

INSERT cards have been included as options for two reasons. The first and less important reason is that if one knows that one or several particular condensed species will be present among the final equilibrium compositions for the first assigned point, then a small amount of computer time can be saved by using an INSERT card. Those condensed species whose chemical formulas are included on an INSERT card will be considered by the program during the initial iterations for the first assigned point. If the INSERT card were not used, only gaseous species would be considered during the initial iterations. However, after convergence, the program would automatically insert the appropriate condensed species and reconverge. Therefore, it usually is immaterial whether or not INSERT cards are used. For all other assigned points the inclusion of condensed species is handled automatically by the program.

The second and more important reason for including the INSERT card option is that, in rare instances, it is impossible to obtain convergence for assigned enthalpy problems (HP or RKT) without the use of an INSERT card. This occurs when, by considering gases only, the temperature becomes extremely low (say several deg K). In these rare cases, the use of an INSERT card containing the name of the required condensed species will eliminate this kind of convergence difficulty. When this difficulty occurs, an error message is generated. This message is described in the subsection Description of Error Messages.

3.2.4 Description of Sample Case Input

A completed input data sheet is shown on page 29 for an assigned enthalpy pressure problem (HP). In this table, lines 1 through 6 identify

the start of the thermodynamic data and include, as examples, data for solid phase aluminum. Lines 10 through 13 identify that the reactant components for this problem are kerosene ($C_1H_{1.9423}$) and air ($N_{0.7803}O_{0.2099}Ar_{0.0049}$). The kerosene (fuel) is supplied as liquid at 298.15 deg K with an enthalpy of -5430 cal/gm-mole. The air (oxidant) is gaseous at 350 deg K with an enthalpy of 195.0 cal/gm-mole. The density of the kerosene is specified as 0.773 gm/cc while that of the air is omitted. Lines 15 through 18 are the NAMELISTS $INPT2 input. Here the case is given the code number 1, HP is identified as the problem type, the combustor pressure is set at 1.80 atm, and the MIX matrix is assigned 35 fuel-to-air ratios for test.

3.3 OUTPUT DATA

The output of Program NOXRAT consists of both printed and punched data. The data falls into two main categories: normal output and error messages. The normal output consists of the printed and punched results usually obtained with each run of the program. If any difficulties are encountered in the solution of a case, one or more error messages are printed. These messages are diagnostic statements which describe the nature of the difficulty. They are described in greater detail in subsection 3.3.2.

3.3.1 Normal Output

The normal output from NOXRAT falls into two main categories: printed output for each fuel-to-air ratio for each assigned condition (e.g., pressure); and printed and punched output for each assigned pressure. The normal output from the first category is:

- *a. The chemical formula of each reactant specie.
- *b. The weight fraction of each reactant specie in the total fuel or oxidant.
- *c. The base enthalpy of each reactant in cal/gm-mole.
- *d. The input temperature of each reactant in deg-K.

---

* Also normal output of CEC.

*e. The density of each reactant (if specified in the input) in gm/cc.

*f. The physical state of each of the specified reactants.

*g. The total oxidant to fuel weights ratio.

*h. The per cent fuel in the reactant mixture.

*i. The equivalence ratio of the reactants.

*j. The weight average density of the reaction mixture in gm/cc (printed as zero if the density of any specie is omitted from the input).

*k. The equilibrium pressure in atm.

*l. The equilibrium temperature in deg K.

*m. The sonic velocity of the combustion production mixture in meters/sec.

*n. The mean enthalpy of the combustion products in cal/gram.

*o. The mean entropy of the combustion products in cal/gram-deg K.

*p. The mean molecular weight of the combustion products in grams.

*q. The differential $(\partial V/\partial P)_T$ in cc/atm.

*r. The differential $(\partial V/\partial T)_P$ in cc/deg K.

*s. The mean heat capacity of the combustion products in cal/gram-deg K.

*t. The mean heat capacity ratio (C_P/C_V) of the combustion products.

*u. The mole fraction and chemical formula of each of the combustion products present at equilibrium at a concentration greater than 5×10^{-6}.

v. The mole fraction of each of the species of interest in the nitric oxide kinetic scheme (Refs 4 through 6) and the mole fractions of $C_{(s)}$, CO, CO_2.

w. The mean molecular weight of the combustion products in grams.

x. The adiabatic flame temperature of the combustion products in deg K.

y. The assigned inlet pressure in atm.

z. The fuel-to-air weight ratio of the reactants.

z1. The atomic composition, inlet temperature (in deg K) and enthalpy (cal/gm-mole) of both the fuel(s) and the oxidant(s).

---

* Also normal output of CEC.

With the exception of the descriptive characteristics of the fuel(s) and oxidant(s) (output #21), the output from this category is clearly labeled and requires no further discussion.

The fuel and oxidant are described by seven characteristic numbers, the first five of which give the atomic composition while the sixth and seventh are the enthalpy in cal/gm-mole at the inlet temperature in deg K. These two lines of output appear directly below the fuel-to-air ratio with the first line always referring to the fuel and the second to the oxidant. Since the fuel used in this analysis has been assumed to be of the form C_xH_y, the first two figures printed describing the fuel are "x" and "y" while the third, fourth, and fifth figures are printed as zero. In this analysis, the oxidant has been taken to be air comprised of nitrogen, oxygen, and argon with the equivalent chemical formula $N_AO_BAr_C$. Hence, the first three numerals printed describing the oxidant are "A", "B", and "C" respectively. The fourth and fifth figures are printed as zero; inclusion of other trace components in the air will change these latter digits accordingly. Further description of this output is included in Appendix IV. The output for the sample data case corresponding to this category of the output is shown on pages 30 and 31.

The normal output for the second category is:

a. The atomic composition of the fuel (C_xH_y).
b. The inlet air temperature in deg ...
c. A code number identifying the set of kinetic constants used in the NO rate formation calculations (see Appendix V).
d. The assigned pressure in atm.
e. The stoichiometric fuel-to-air ratio.
f. For each fuel-to-air ratio specified. the program prints and punches two lines of output containing twelve items of data. This data is (consecutively): the mixture ratio (mass fuel to mass fuel and air); the equivalence ratio; the density of the combustion products in gm/cm^3; the adiabatic flame temperature of the combustion products in deg K; the equilibrium mole fraction of NO, CO,

$C_{(s)}$, and CH_2 (unburned hydrocarbons). and the kinetic parameters R_1, R_6 (in gm-moles/cm^3-sec), K_1, and K_2 (dimensionless). The output for the sample data case corresponding to this category of the output is shown on page 32.

Program NOXRAT prints intermediate output for each input set of REACTANT cards and for each fuel-to-air ratio. The former consists of a listing of the input data for the case and a listing of the species being considered as products of the combustion process. The latter data is the result of intermediate calculations within NOXRAT and is not described here. It is generally not of any interest to the user; however, the output for one fuel-to-air ratio for the sample data case is shown on page 33.

3.3.2 Description of Error Messages

The known error messages in Program NOXRAT* are:

a. In rare instances, it is impossible to obtain convergence for assigned enthalpy problems (HP or RKT) without the use of an INSERT card. This occurs when, by considering gases only, the temperature becomes extremely low (say several deg K). In these rare cases, the use of an INSERT card containing the name of the required condensed species will eliminate this kind of convergence difficulty. When this difficulty occurs, the following message is printed by the program: "LOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE BEEN INCLUDED ON AN INSERT CARD".

b. If the user mixes the order of the cards for a particular species in the thermodynamic data file, the program will print: "ERROR IN ORDER OF DATA CARDS FOR --------(specie name)". This is a nonfatal error and the program will continue to execute, however, the specie in error will be deleted from the thermodynamic inventory.

c. If there are cards in the input data deck that do not belong, the program will write the card and: "ERROR IN ABOVE CARD. IGNORE CONTENTS". This is a nonfatal error to the program, but causes it to skip to the next data set.

---

* These are as those for CEC.

d. If there are errors in the REACTANTS data cards the program will write: "ERROR IN REACTANT CARDS". This is a nonfatal error to the program but causes it to skip to the next data set.

e. If the convergence tests are not satisfied for the equilibrium products the program will print: "ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREMENTS FOR THE POINT ____".

f. If the temperature calculated for the combustion is out of the range of the thermodynamic data the program will print: "THE TEMPERATURE = ______ IS OUT OF RANGE FOR POINT ____".

g. If the phases of a condensed specie are out of order, the program will print: "PHASES OF A CONDENSED SPECIE ARE OUT OF ORDER".

3.4 MISCELLANEOUS OPERATIONAL INFORMATION

Program NOXRAT occupies approximately 71,000 core locations during loading and approximately 63,000 core locations during execution on the CDC 6600 computer. Actual program length is approximately 38,000 core locations. Hence, the total storage requirement for this program is comfortably within the CDC 6600 core capacity of 131,000 locations.

The execution time of Program NOXRAT depends primarily upon the number of assigned pressure levels and upon the number of fuel-to-air ratios at each of the pressure levels to be tested. A typical operating condition of one assigned pressure and 35 fuel-to-air ratios requires approximately 66 systems seconds (central processor time is approximately 52 secs) for execution. Each succeeding point at any given pressure and any selected fuel-to-air ratio will require approximately one second of over-all machine time.

A "scratch" tape is required by the program. This scratch tape number is not assigned a Fortran name but is given the value of 4 by the program. The instructions necessary for mounting this tape must be supplied to the computer/computer operator upon submission of a run.

NORTHERN RESEARCH AND ENGINEERING CORPORATION

3.5 DATA INPUT SHEET

ENGINEER: RDS **PROJECT:** NOx from Gas Turbine Combustors **PROJECT NO:** 1162

TITLE: Sample to Illustrate the Use of Program NOXRAT **SHEET:** 1 **OF** 1

LOCATION

	1–72	
Line 1	THERMO	
Line 2	300.000 1000.000 5000.000	
Line 3	AL(S) J12/65AL 1.0 00 00 0S 300.00 933.000	1
Line 4	0. 0. 0. 0. 0.	2
Line 5	0. 0. 0.22258601E-01 0.25561698E-02 0.25963942E-06	3
Line 6	-0.44923993E-08 0.38348586E-11-0.77250039E+03-0.10016767E+01	4
Line 7		
Line 8		
Line 9		
Line 10	REACTANTS	
Line 11	C 1. H 1.9423 1.0 -5430. L298.15 F .773	
Line 12	N .7803 O .2099 AR.0049 1.0 195.0 G350.00 0	
Line 13		
Line 14	NAMELISTS	
Line 15	$INPT2 KASE=1,HP=T,P=1.80,FA=T,MIX=.0008494,.006795,.01699,.02718,.03398,	
Line 16	.03737,.04077,.04417,.04757,.05096,.05436,.05776,.06116,.06455,.06795,.07135,	
Line 17	.07475,.07814,.08154,.08494,.08834,.09173,.09513,.09853,.1019,.1087,.1189,	
Line 18	.1291,.1393,.1495,.1597,.1699,.1801,.1903,.2005 $	

3.6 SAMPLE CASE OUTPUT

```
                         THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO.   1
                                                              WT FRACTION  ENTHALPY  STATE   TEMP     DENSITY
           CHEMICAL FORMULA                                   (SEE NOTE)   CAL/MOL           DEG K    G/CC
FUEL     C  1.00000   H  1.94230                               1.00000    -5430.000    L     298.15    .7730
OXIDANT  N   .78030   O   .20990   AR  .00490                  1.00000      195.000    G     350.00   -0.0000

         O/F=  5.2549   PERCENT FUEL= 15.9876   EQUIVALENCE RATIO=  2.7929   DENSITY=  0.0000

THERMODYNAMIC PROPERTIES

P, ATM               1.8000
T, DEG K               1184
H, CAL/G              -50.8
S, CAL/(G)(K)        2.4465

M, MOL WT            22.018
(DLV/DLP)T         -1.00236
(DLV/DLT)P           1.0288
CP, CAL/(G)(K)        .3974
GAMMA (S)            1.3123
SON VEL,M/SEC         766.1

MOLE FRACTIONS

AR                   .00626
CH4                  .00061
CO                   .24395
CO2                  .00742
HCN                  .00001
H2                   .23416
H2O                  .00929
NH3                  .00003
N2                   .49827

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)      C         CH        CH2       CH3       CN        CN2       C2        C2H       C2H2
C2H4      C2N       C2N2      C2O       C3        C3O2      H         HCO       HO2       H2O(S)
H2O(L)    N         NH        NH2       NO        NO2       N2C       N2H4      N2O       N2O4
O         OH        O2

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS
```

OUTPUT FROM OUT3

```
C(S)           0.
CO             2.43954611E-01
CO2            7.41718910E-03
H              5.26478295E-08
N              0.
NO             0.
N2O            0.
O              0.
O2             0.
OH             0.
MOLEC. WT.     2.20178947E+01
TEMP.(K)       1.18428579E+03
PRESS.(ATM)    1.80000000E+00
FUEL AIR RAT.  1.90300000E-01
 1.00000000E+00 1.94230000E+00-0.                -0.            -0.              -5.43000000E+03 2.98150000E+02
 7.80300000E-01 2.09900000E-01 4.90000000E-03-0.                -0.              1.95000000E+02 3.50000000E+02
```

OUTPUT FROM RATES

```
FUEL= C 1.00000000E+00H 1.94230000E+00 INLET AIR T.(K)=  3.50000000E+02
PRESS.(ATM)=  1.80000000E+00ICODE=  1PHI STOICH.=  6.79522849E-02
-8.49679E-04 1.24999E-02 1.62731E-03 3.90469E+02 0.          0.
 0.          3.36136E-06 0.          0.          1.00000E+35 1.00000E+35
 6.74914E-03 9.99966E-02 1.00034E-03 6.35172E+02 6.40730E-08 0.
 0.          2.67302E-05 0.          0.          1.00000E+35 1.00000E+35
 1.67062E-02 2.50028E-01 6.27465E-04 1.01256E+03 3.41444E-05 0.
 0.          6.61614E-05 0.          0.          1.00000E+35 1.00000E+35
 2.64608E-02 3.99987E-01 4.71210E-04 1.34823E+03 9.38710E-04 4.47846E-08
 0.          1.04785E-04 0.          5.68904E-15 1.00000E+35 1.33333E+00
 3.28433E-02 5.00057E-01 4.08777E-04 1.55405E+03 1.15681E-03 1.60756E-06
 0.          1.30132E-04 0.          6.35516E-13 1.00000E+35 8.44145E-01
 3.60239E-02 5.49945E-01 3.84573E-04 1.65178E+03 1.45298E-03 7.04703E-06
 0.          1.42640E-04 0.          3.78222E-12 1.00000E+35 7.42706E-01
 3.91729E-02 5.99980E-01 3.63656E-04 1.74667E+03 2.21656E-03 2.46379E-05
 0.          1.55097E-04 0.          1.70770E-11 1.00000E+35 6.43491E-01
 4.23015E-02 6.50015E-01 3.45472E-04 1.83838E+03 2.81087E-03 7.44642E-05
 0.          1.67465E-04 0.          6.09179E-11 1.00000E+35 5.48862E-01
 4.54099E-02 7.00050E-01 3.24566E-04 1.92673E+03 3.38840E-03 1.99926E-04
 0.          1.79735E-04 0.          1.77069E-10 1.00000E+35 4.60009E-01
 4.84890E-02 7.49518E-01 3.15653E-04 2.01099E+03 [illegible]88817E-03 4.85274[illegible] 04
 0.          1.91859E-04 0.          4.25301E-10 1.00000E+35 3.[illegible]729E-01
 5.15573E-02 7.99973E-01 3.03440E-04 2.09076E+03 4.24244E-03 1.04687E-03
 0.          2.03885E-04 0.          8.56118E-10 1.00000E+35 3.01751E-01
 5.46060E-02 8.50008E-01 2.92863E-04 2.16427E+03 4.37220E-03 2.26136E-03
```

0.	2.15741E-04	0.	1.42201E-09	1.00000E+35	2.32452E-01
5.76350E-02	9.00043E-01	2.83910E-04	2.22916E+03	4.20475E-03	4.40149E-03
0.	2.27367E-04	5.46340E-08	1.90261E-09	3.02085E-01	1.70120E-01
6.00359E-02	9.49931E-01	2.76696E-04	2.28188E+03	3.69903E-03	8.04012E-03
0.	2.38654E-04	8.32856E-08	1.95574E-09	2.72042E-01	1.15653E-01
6.36266E-02	9.99966E-01	2.71407E-04	2.31796E+03	2.88281E-03	1.38758E-02
0.	2.49539E-04	9.30193E-08	1.43131E-09	2.34000E-01	7.03456E-02
6.65982E-02	1.05000E+00	2.68388E-04	2.33169E+03	1.92620E-03	2.24962E-02
0.	2.59854E-04	7.08682E-08	6.84926E-10	1.92441E-01	3.70303E-02
6.95511E-02	1.10004E+00	2.67678E-04	2.32155E+03	1.11403E-03	3.37040E-02
0.	2.69537E-04	3.69222E-08	2.17679E-10	1.53401E-01	1.71780E-02
7.24767E-02	1.14992E+00	2.68632E-04	2.29452E+03	6.00371E-04	4.61581E-02
0.	2.79666E-04	1.51082E-08	5.50369E-11	1.21971E-01	7.86007E-03
7.53925E-02	1.19996E+00	2.70474E-04	2.25922E+03	3.19914E-04	5.86741E-02
0.	2.87448E-04	5.56804E-09	1.29702E-11	9.63835E-02	4.46745E-03
7.82900E-02	1.24999E+00	2.72751E-04	2.22069E+03	1.72782E-04	7.06175E-02
0.	2.95944E-04	1.98518E-09	3.06530E-12	8.08468E-02	1.65345E-03
8.11695E-02	1.30003E+00	2.75267E-04	2.18109E+03	9.48818E-05	8.17934E-02
0.	3.04196E-04	0.	0.	1.00000E+35	1.00000E+35
8.40226E-02	1.34992E+00	2.77926E-04	2.14147E+03	5.29427E-05	9.21413E-02
0.	3.12217E-04	0.	0.	1.00000E+35	1.00000E+35
8.68664E-02	1.39995E+00	2.80707E-04	2.10200E+03	2.98155E-05	1.01755E-01
0.	3.20045E-04	0.	0.	1.00000E+35	1.00000E+35
8.96926E-02	1.44999E+00	2.83583E-04	2.06297E+03	1.69237E-05	1.10663E-01
0.	3.27676E-04	0.	0.	1.00000E+35	1.00000E+35
9.24766E-02	1.49958E+00	2.86522E-04	2.02481E+03	9.70306E-06	1.18863E-01
0.	3.35055E-04	0.	0.	1.00000E+35	1.00000E+35
9.80428E-02	1.59965E+00	2.92709E-04	1.94949E+03	3.17714E-06	1.33771E-01
0.	3.49412E-04	0.	0.	1.00000E+35	1.00000E+35
1.06265E-01	1.74976E+00	3.02670E-04	1.84064E+03	5.87166E-07	1.52916E-01
[illegible]	3.69735E-04	0.	0.	1.00000E+35	1.00000E+35
[illegible].339E-01	1.89986E+00	3.13547E-04	1.73632E+03	1.02779E-07	1.69302E-01
0.	3.88770E-04	0.	0.	[illegible].00000E+35	1.00000E+35
1.22268E-01	2.04997E+00	3.25478E-04	1.63605E+03	1.64228E-08	1.83789E-01
0.	4.06719E-04	0.	0.	1.00000E+35	1.00000E+35
1.30057E-01	2.20007E+00	3.38634E-04	1.53937E+03	0.	1.96964E-01
0.	4.23828E-04	0.	0.	1.00000E+35	1.00000E+35
1.37708E-01	2.35018E+00	3.53224E-04	1.44587E+03	0.	2.09262E-01
0.	4.40828E-04	0.	0.	1.00000E+35	1.00000E+35
1.45226E-01	2.50028E+00	3.69517E-04	1.35514E+03	0.	2.21042E-01
0.	4.62013E-04	0.	0.	1.00000E+35	1.00000E+35
1.52614E-01	2.65039E+00	3.87821E-04	1.26699E+03	0.	2.32622E-01
0.	5.26076E-04	0.	0.	1.00000E+35	1.00000E+35
1.59876E-01	2.80049E+00	4.07827E-04	1.18429E+03	0.	2.43955E-01
0.	1.10630E-03	0.	0.	1.00000E+35	1.00000E+35
1.67014E-01	2.95060E+00	4.20324E-04	1.14008E+03	0.	2.46168E-01
5.68296E-03	4.69200E-03	0.	0.	1.00000E+35	1.00000E+35

	FUEL	OXIDANT	MIXTURE
H,CAL/G	-3.88719820E+02	1.34636455E+01	-5.08357020E+01
V+	4.25394067E-01	0.	6.80101579E-02
V-	0.	-2.89848123E-02	-2.43508462E-02
ATOMS/G			
C	7.15874437E-02	0.	3.14450899E-02
H	1.39044292E-01	0.	2.22297982E-02
N	0.	5.38752954E-02	4.52619469E-02
O	0.	1.44924061E-02	1.21754231E-02
AR	0.	3.38317246E-04	2.84228553E-04

PT	C	H	N	O	AR						
1	-2.832	-.000	-9.396	-.000	-12.706	-.000	-35.262	-.000	-24.674	-.000	15.000

4. REFERENCES

1. Caretto, L. S., Sawyer, R. F., and Starkman, E. S., The Formation of Nitric Oxide in Combustion Process, Presented at 1968 Technical Meeting, Central States Section, The Combustion Institute, March 26-27, 1968.

2. Bartok, W., et al, Systems Study of Nitrogen Oxide Control Methods for Stationary Sources (Esso Report No. GR-1-NOS-69), Interim Status Report to National Air Pollution Control Administration, Esso Research and Engineering Company, May, 1969.

3. Newhall, H. K., Kinetics of Engine-Generated Nitrogen Oxides and Carbon Monoxide, Presented at the Twelfth Symposium (International) on Combustion, The Combustion Institute, 1968.

4. Lavoie, G. A., Heywood, J. B., and Keck, J. C., Experimental and Theoretical Study of Nitric Oxide Formation in Internal Combustion Engines (Publication No. 69-10), Fluid Mechanics Laboratory, Massachusetts Institute of Technology, Cambridge, Mass., November, 1969, published in Combustion Science and Technology, vol. 1, 1970, pp. 316-326.

5. Lavoie, G. A., Nitric Oxide Measurements in an Internal Combustion Engine by Visible and Near Infra-Red Emission Spectroscopy, ScD Thesis, Massachusetts Institute of Technology, Cambridge, Mass., February, 1970.

6. Heywood, J. B., Fay, J. A., and Linden, L. H., Jet Aircraft Air Pollutant Production and Dispersion (AIAA Paper No. 70-115), American Institute of Aeronautics and Astronautics, Presented at AIAA 8th Aerospace Sciences Meeting, New York, N. Y., January 19-21, 1970.

7. Schofield, K., "An Evaluation of Kinetic Rate Data for Reactions of Neutrals of Atmospheric Interest", Planetary and Space Science, vol. 15, 1967, pp. 643-670.

8. Campbell, I. M., and Thrush, B. A., "Reactivity of Hydrogen to Atomic Nitrogen and Atomic Oxygen", Transactions of the Faraday Society, vol. 15, 1968, pp. 1265-1274.

9. Baulch, D. L., et al, Critical Evaluation of Rate Data for Homogeneous, Gas Phase Reactions of Interest in High-Temperature Systems, School of Chemistry, The University, Leeds, England, 1969.

10. Zeleznik, F. J., and Gordon, S., A General IBM 704 or 7090 Computer Program for Computation of Chemical Equilibrium Compositions, Rocket Performance, and Chapman-Jouquet Detonations (NASA TN D-1454), National Aeronautics and Space Administration, October, 1963.

11. Gordon, S., and Zeleznik, F. J., A General IBM 704 or 7090 Computer Program for Computation of Chemical Equilibrium Compositions, Rocket Performance, and Chapman-Jouquet Detonations, Supplement I - Assigned Area-Ratio Performance (NASA TN D-1737), National Aeronautics and Space Administration, October, 1963.

12. Zeleznik, F. J. and Gordon, S., "Calculation of Complex Chemical Equilibrium", Industrial and Engineering Chemistry, vol. 60, no. 6, June, 1968, pp. 27-57.

13. Gordon, S. and McBride, B., Preliminary Description of CEC, A Computer Program for the Calculation of Chemical Equilibrium Compositions with Applications, NASA Lewis Research Center, November 19, 1968.

14. Gordon, S. and McBride, B. J., Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouquet Detonations (NASA SP-273), National Aeronautics and Space Administration, Washington, D. C., 1971.

15. McBride, B. J. and Gordon, S., Fortran IV Program for Calculation of Thermodynamic Data (NASA Technical Note, NASA TN D-4097), National Aeronautics and Space Administration, Lewis Research Center, Cleveland, Ohio, 1967.

16. Chao, J., et al, Janaf Thermochemical Tables (PB 168 370, PB 168 370-1, PB 168 370-2, and PB 168 370-3), Dow Chemical Company, Midland, Mich., August, 1965.

17. Lavoie, G. A., "Spectroscopic Measurement of Nitric Oxide in Spark Ignition Engines", Combustion and Flame, vol. 15, 1970, pp. 97-108.

18. Fletcher, R. S. and Heywood, J. B., A Model for Nitric Oxide Emissions from Aircraft Gas Turbine Engines (AIAA Paper No. 71-123), American Institute of Aeronautics and Astronautics, AIAA 9th Aerospace Sciences Meeting, New York, N. Y., January 25-27, 1971.

5. TABLES

TABLE I

KINETIC DATA FOR THE NITRIC OXIDE REACTION SCHEME

	Reaction No.	A_i (cm^3/sec gm-mole deg K)	n_i	E_i (kcal/gm-mole)
ICODE = 1 (from Refs 4, 5)	1	1.2046×10^{13}	0.0	0.0
	2	1.2046×10^{13}	0.0	7.1
	3	4.2161×10^{13}	0.0	0.0
	4	3.0115×10^{13}	0.0	10.8
	5	3.6138×10^{13}	0.0	24.0
	6	4.8184×10^{13}	0.0	24.0
ICODE = 2 (from Refs 9,17)	1	3.1×10^{13}	0.0	0.334
	2	6.4×10^{9}	1.0	6.25
	3	4.1×10^{13}	0.0	0.0
	4	2.9513×10^{13}	0.0	10.77
	5	3.8146×10^{13}	0.0	24.1
	6	4.5775×10^{13}	0.0	24.1
ICODE = 3 (from Ref 18)	1	3.0717×10^{13}	0.0	0.33
	2	1.3251×10^{10}	1.0	7.1
	3	4.2161×10^{13}	0.0	0.0
	4	2.9513×10^{13}	0.0	10.77
	5	3.8146×10^{13}	0.0	24.1
	6	4.5775×10^{13}	0.0	24.1
ICODE = 4 (from Ref 18)	1	1.0239×10^{13}	0.0	0.0
	2	3.7945×10^{12}	0.0	7.0
	3	4.1559×10^{13}	0.0	0.0
	4	2.9513×10^{13}	0.0	10.77
	5	3.8146×10^{13}	0.0	24.1
	6	4.5775×10^{13}	0.0	24.1

where

$$k = A_i T^{n_i} \exp(-E_i/RT)$$

T = Temperature in deg K

$R = 1.987 \times 10^{-3}$ kcal/gm-mole deg K

TABLE 2 - PROGRAM OR SUBPROGRAM FUNCTION

Program or Subprogram	Description
NOXRAT	Main program to calculate chemical equilibrium compositions with applications; the main program controls the calculation and directs the input and output
REACT	Subroutine to read and convert reaction input data
SEARCH	Subroutine to search tape for thermodynamic data for species to be considered
EQULBRM	Subroutine to calculate equilibrium composition and properties
CPHS	Subroutine to calculate thermodynamic properties for individual species
MATRIX	Subroutine to perform matrix inversion
MGAUSD	Subroutine to solve any linear set of up to 20 equations
VARFMT	Subroutine to set variable formats
OUT1	Subroutine to write output
OUT2	Subroutine to write output
OUT3	Subroutine to write output
HCALC	Subroutine to calculate enthalpy for propellant using coefficients
MOLIER	Subroutine to calculate thermodynamic equilibrium properties at assigned temperatures and pressures
CMBSTN	Subroutine to calculate theoretical thermodynamic combustion properties
DETON	Subroutine to calculate Chapman-Jouguet detonations
SHCK	Subroutine to terminate program if a shock occurs
ROCKET	Subroutine to calculate rocket performance

TABLE 2 - PROGRAM OR SUBPROGRAM FUNCTION (CONTINUED)

Program or Subprogram	Description
RKTOUT	Subroutine to write output for rocket performance
RATIO	Subroutine to interpolate area ratio
SET	Subroutine to interpolate area ratio
FROZEN	Subroutine to calculate frozen composition expansion only
RATES	Subroutine to calculate rate constants for the NO reaction scheme

6. FIGURES

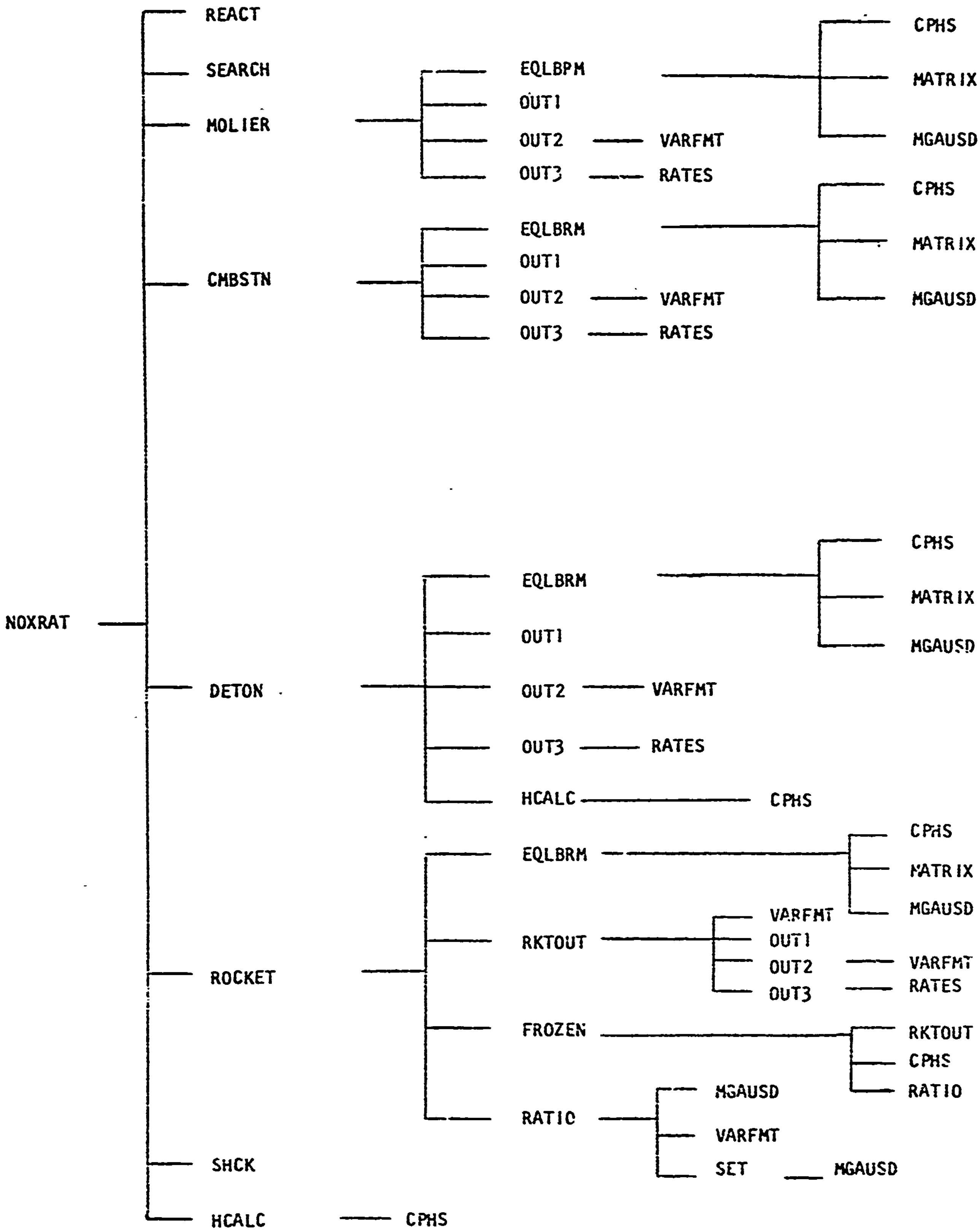

FIGURE 1 - MODULAR TREE DIAGRAM

7. NOMENCLATURE

Symbol	Description	Units
C_p	Specific heat at constant pressure	cal/gm-deg K
C_V	Specific heat at constant volume	cal/gm-deg K
P	Pressure	atm
T	Temperature	deg K
V	V[illegible]	cc

8. APPENDICES

APPENDIX I - OVER-ALL PROGRAM LOGIC

The over-all computer flow of NOXRAT is identical to that of CEC excepting the additional CALL to Subroutine RATES by Subroutine OUT3. The other modifications to OUT3 and to the main program (NOXRAT) do not affect the over-all program logic. A complete description of the program logic is available in References 11, 13, 14, and 15. A modular diagram of NOXRAT is provided as Figure 1 (Ref 13). Table 2 contains a brief statement as to the role of each routine in the program.

APPENDIX II - COMMON FORTRAN NOMENCLATURE

The following tables contain the COMMON Fortran nomenclature for Program NOXRAT that was added to that of Program CEC. COMMON consists of labeled blocks; the nomenclature is arranged in alphabetical order for each block. The metric system of units is included in the nomenclature.

Nomenclature for COMMON/SNEW

Fortran Symbol	Symbol	Description	Units
INDFA		Index of equivalence ratios	
RON	F/A	Fuel-to-air mass ratio	

Nomenclature for COMMON/DICK

Fortran Symbol	Symbol	Description	Units
ATT(J,I)	T_j	jth value of the adiabatic flame temperature (in the combustor) at a particular fuel-to-air mass ratio i	deg K
BCON1(J,I)	$y_{C_{(s)j}}$	Equilibrium mole fraction of carbon at the jth pressure level at a particular fuel-to-air mass ratio i	
BCON2 (J,I)	y_{CO_j}	Equilibrium mole fraction of carbon monoxide at the jth pressure level at a particular fuel-to-air mass ratio i	
BCON6(J,I)	y_{NO_j}	Equilibrium mole fraction of nitric oxide at the jth pressure level at a particular fuel-to-air mass ratio i	
CH2(J,I)	$y_{CH_{2_j}}$	Equilibrium mole fraction of unburned hydrocarbons in the combustion products (excluding $C_{(s)}$ and CO) expressed as CH2 at the jth pressure level at a particular fuel-to-air mass ratio i	

Fortran Symbol	Symbol	Description	Units
EK1(J,I)	$(K_1)_j$	Ratio of forward reaction rate at the ith pressure level for a particular fuel-to-air mass ratio i	
EK2(J,i)	$(K_2)_j$	Ratio of forward reaction rate at the jth pressure level for a particular fuel-to-air mass ratio i	
F(I)	F	Mixture ratio	
MIX(I)		Matrix of specified fuel-to-air mass ratios	
PHI(I)	Φ	Equivalence ratio	
ROH(J,I)	ρ_j	Equilibrium density at the jth pressure level at a particular fuel-to-air mass ratio i	gm/cm^3
R1(J,I)	$(R_1)_j$	Forward reaction rate for the first reaction at the jth pressure level at a particular fuel-to-air mass ratio i	$gm\text{-}mole/cm^3\text{-}sec$
R6(J,I)	$(R_6)_j$	Forward reaction rate for the sixth reaction at the jth pressure level at a particular fuel-to-air mass ratio i	$gm\text{-}mole/cm^3\text{-}sec$

APPENDIX III - MAIN ROUTINE - NOXRAT

The changes to the main routine of CEC are as follows:

a. The main program was renamed NOXRAT, thus replacing the CEC name "MAIN".

b. The subscripted variable MIX was expanded from 15 to 50. MIX is the matrix of specified fuel-to-air ratios.

c. Labeled COMMON blocks SNEW, DICK, and EQNEW were added. Definitions of the variables contained in these blocks are povided in Appendix II.

d. The statement DO 303 I = 1, 15 was modified to DO 303 I = 1, 50. This is consistent with the expansion of the MIX matrix from 15 to 50.

e. Statement number 322:DO 625 IST = 1, 15 was modified to read DO 625 IST = 1, 40. This is consistent with the decision to limit each set of specified fuel-to-air ratios to between 35 and 40 entries.

f. The statement INDFA = IST was inserted directly after the statement numbered 322. The statement RON = MIX(IST) was inserted directly after the statement numbered 323. Both of these new variables are part of the new labeled COMMON blocks and are used only in Subroutine RATES.

APPENDIX IV - SUBROUTINE OUT3

Subroutine OUT3 is an entry point to Subroutine OUT1. The main purpose of this subroutine had been to provide the written output for the CEC program. The modifications incorporated into OUT3 permit identification of the species of interest in the kinetic scheme (previously described). Once identified, these variables are transmitted to Subroutine RATES by means of COMMON and a call statement from OUT3. The specific changes to OUT3 are as follows:

a. The subscripted variable MIX was expanded from 15 to 50. MIX is the matrix of specified fuel-to-air ratios.

b. A dimension statement was added for the variables "SIEGEL" and "CONCKI". "SIEGEL" is a singly-subscripted variable containing the alphanumeric characters used in the idenfification of the chemical species of interest in the kinetic scheme. The variable "CONCKI" is a doubly-subscripted array representing the equilibrium mole fraction of a given species for a particular pressure level at a specified fuel-to-air ratio.

c. Labeled COMMON blocks SNEW, DICK, and EQNEW were added. Definitions of the variables contained in these blocks are provided in Appendix II.

d. The elements of the "SIEGEL" array were entered into the program via a DATA statement.

e. Statement number 1000 was changed from a RETURN statement to a CONTINUE statement.

f. 34 statements were added to the program after statement number 1000 in order to identify which elements of the CEC array EN (containing the moles of a given species present in a particular reaction mixture) were the ones of interest in the kinetic analysis. This problem was created by the storage of the alphanumeric characters identifying reaction species in the CEC generated array

"SUB". This array was created in such a manner that determination of the specific elements of interest to NREC had to be accomplished by a direct comparison of the alphanumeric data in the "SUB" array with the specific names in the input "SIEGEL" array. This comparison and the calculation of the equilibrium mole fractions was accomplished in the DO 3000 loop of OUT3. The remaining statements added to OUT3 allow the equilibrium mole fractions and names of the species of interest, the molecular weight and adiabatic flame temperature of the combustion products, the assigned pressure, the fuel-to-air ratio, and the atomic and thermal characteristics of the fuel and oxidant to be printed for each specified fuel-to-air ratio. This output appears directly beneath the "normal" output (i.e., regular CEC type) generated by OUT3. The final cards added to OUT3 are the CALL statement to Subroutine RATES and the Subroutine RETURN statement.

APPENDIX V - SUBROUTINE RATES

The primary function Subroutine RATES is to produce data, in the form of a deck of cards, which specify all of the kinetic properties required by Program GASNOX* at the equilibrium combustor conditions.

Subroutine RATES is called by Subroutine OUT3 of Program NOXRAT; it does not call any other subroutines. Subroutine RATES does not require external input but does provide external output in the form of punch cards and paper. Internal input and output are transmitted as arguments of the subroutine and through COMMON. The internal input consists of:

A	ANUM	CONCKI	E	EN
ENTH	ICODE	INDFA	MIX	NPT
NREAC	PPP	RON	RTEMP	TTT
WM				

The internal output consists of:

ATT	BCON1	BCON2	BCON6	CH2
EK1	EK2	F	PHI	RON
R1	R6			

The external output consists of:

ANUM	ATT	BCON1	BCON2	BCON6
CH2	EKS	EK1	EK2	F
ICODE	PHI	PPP	RON	RTEMP
A1	R6			

Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols used in Subroutine RATES which are not included in COMMON.

Fortran Symbol	Symbol	Description	Units
A(I)	A_i	Pre-exponential factors in the kinetic equations	cm^3/sec-gm mole deg K
ANUM(I,J)	$a_{i,j}$	Atomic number $a_{1,1}$ = carbon $a_{1,2}$ = hydrogen $a_{2,2}$ = oxygen	

* See Volume 3.

Fortran Symbol	Symbol	Description	Units
CONCKI(J,I)	$y_{i,j}$	Equilibrium mole fraction of the ith species for the jth pressure at a particular fuel-to-air mass ratio i	
CONMCM(K,J,I)	$(y_i)_j$	Equilibrium concentration of the kth species for the jth pressure at a particular fuel-to-air mass ratio i	gm moles/cm^3
E(I)	E_i	Activation energies for the kinetic equations	kcal/gm-mole
EKS	k_s	Fuel-to-air mass ratio at stoichiometric conditions	
EN(I)	n_i	Temperature exponent for the kinetic equations	
ENTH(N)	H_n	Enthalpy of reactant n	cal/gm-mole
ICODE		Indicator ICODE = 1 if kinetic rate constants of Lavoie are employed (Refs 4, 5) ICODE = 2 if "best" kinetic data are employed (Refs 9, 17) ICODE = 3 if "high" kinetic data selected from Reference 18 are employed ICODE = 4 if "low" kinetic data selected from Reference 18 are employed	
IPRINT		Indicator IPRINT = 0 if data is not to be printed and punched IPRINT = 1 if data is to be printed and punched	
IST		Index of equivalence ratios	
NPT		Index of pressures	
NREAC	n_{react}	Number of the nth reactant species	
PPP(J)	P_j	jth value of the pressure in the combustor	atm

Fortran Symbol	Symbol	Description	Units
RATEK(K,J,I)	$(k_k)_j$	jth value of the reaction rate for the kth kinetic equation at a particular fuel-to-air mass ratio i	cm^3/sec-gm mole
RATWTS		Ratio of atomic numbers	
RTEMP(N)	T_n	Inlet temperature of reactant n	deg K
R2(J,I)	$(R_2)_j$	Forward Reaction rate for the second reaction at the jth pressure level at a particular fuel-to-air mass ratio i	gm-mole/cm^3-sec
R3(J,I)	$(R_3)_j$	Forward reaction rate for the third reaction at the jth pressure level at a particular fuel-to-air mass ratio i	gm-mole/cm^3-sec
R4(J,I)	$(R_4)_j$	Forward reaction rate for the fourth reaction at the jth pressure level at a particular fuel-to-air mass ratio i	gm-mole/cm^3-sec
R5(J,I)	$(R_5)_j$	Forward reaction rate for the fifth reaction at the jth pressure level at a particular fuel-to-air mass ratio i	gm-mole/cm^3-sec
TTT(J)	T_j	jth value of the temperature (in the combustor) at a particular fuel-to-air mass ratio	deg K
WM(J,I)	MW_j	jth value of the molecular weight of the reaction products at a particular fuel-to-air mass ratio	gm/gm-mole

Analysis Procedure

The step-by-step procedure of Subroutine RATES is given below. At the conclusion of the step-by-step procedure, the Fortran listing of the subroutine appears:

a. Establish the printing and punching control.

b. Convert equilibrium mole fractions of $C_{(s)}$, CO, CO_2, H, N, NO, N_2O, O, O_2 to moles/cm^3 by the relationship

$$(y_i)_j = [y_{i,j}][P_j/82.057T_j]$$

c. Compute the forward reaction rate constants as

$$(k_i)_j = A_i T_j^n \exp[-E_i/RT_j]$$

d. Calculate $(R_1)_j$, $(R_2)_j$, $(R_3)_j$, $(R_4)_j$, $(R_5)_j$, and $(R_6)_j$

$$(R_1)_j = (k_1)_j (N_e)_j (NO_e)_j$$

$$(R_2)_j = (k_2)_j (N_e)_j (O_{2e})_j$$

$$(R_3)_j = (k_3)_j (N_e)_j (OH_e)_j$$

$$(R_4)_j = (k_4)_j (H_e)_j (N_2O_e)_j$$

$$(R_5)_j = (k_5)_j (O_e)_j (N_2O_e)_j$$

$$(R_6)_j = (k_6)_j (O_e)_j (N_2O_e)_j$$

e. Compute $(K_1)_j$ and $(K_2)_j$

$$(K_1)_j = (R_1)_j/[(R_2)_j + (R_3)_j]$$

$$(K_2)_j = (R_6)_j/[(R_4)_j + (R_5)_j]$$

If $(R_2)_j$ and $(R_3)_j$ equal zero, $(K_1)_j = 10^{35}$

If $(R_4)_j$ and $(R_5)_j$ equal zero, $(K_2)_j = 10^{35}$

f. Compute ρ_j as

$$\rho_j = P_j MW_j/82.057T_j$$

g. Compute k_s as

$$k_s = \frac{(12a_{1,1} + 1a_{1,2})a_{2,2}}{28.99\left(a_{1,i} + \frac{a_{1,2}}{4}\right)}$$

h. Compute Φ as

$$\Phi = \frac{F/A}{k_s}$$

i. Compute F as

$$F = \Phi k_s/(1 + \Phi k_s)$$

j. Compute $y_{CH_{2j}}$

$$y_{CH_{2j}} = 1\left\{\left[\frac{a_{1,1}/a_{1,2}}{1 + \frac{12a_{1,1}}{a_{1,2}}}\right]\left[\frac{MW_j(F/A)}{(F/A)+1}\right] - y_{CO_j} - y_{CO_{2j}} - y_{C(s)_j}\right\}$$

k. Repeat steps a through j for each of the specified pressure levels.

l. If all of the input fuel-to-air mass ratios have been examined, proceed to step m. If not, return to Subroutine OUT3 of Program NOXRAT and repeat the set of calculations in NOXRAT leading up to the calling of Subroutine RATES.

m. If this is the first fuel-to-air mass ratio at the particular pressure in question, write and punch a heading card. If not, go to step n.

n. Write and punch the required output data at the jth pressure level (for each fuel-to-air mass ratio at that pressure level). This data is: F; ϕ; ρ_j; T_j; $y_{NO,j}$; $y_{CO,j}$; $y_{C_{(s)},j}$; $y_{CH_{2},j}$; $(R_1)_j$, $(R_6)_j$, $(K_1)_j$; and $(K_2)_j$.

o. If this is the last fuel-to-air mass ratio at the jth pressure level, proceed to step p. If not, return to step m at the next ratio.

p. If this is the last pressure specified, proceed to step q. If not, return to step m.

q. Return.

```
      SUBROUTINE RATES(CONCKI,WM,TTT,PPP,ANUM,ENTH,RTEMP,NPT,NREAC)
      REAL MIX(50)
      DIMENSION CONCKI(10,30),TTT(13),PPP(13),WM(13),ANUM(15,5),ENTH(15)
     1,RTEMP(15)
      DIMENSION R2(30,40),R3(30,40),R4(30,40),R5(30,40),RATEK(6,30,40),C
     1ONMCM(10,30,40),A(6),EN(6),F(6)
      COMMON/SNEW/RON,INDFA
      COMMON/DICK/MIX
      COMMON/EQNEW/R1(30,40),R6(30,40),EK1(30,40),EK2(30,40),ROH(30,40),
     1CH2(30,40),ATT(13,40),F(40),PHI(40),BCON1(30,40),BCON2(30,40),BCON
     26(30,40)
      DATA(A(I),I=1,6)/3.1E+13,6.4E+09,4.1E+13,2.9513E+13,3.8146E+13,4.5
     1775E+13/,(EN(I),I=1,6)/0.,1.,0.,0.,0.,0./,(E(I),I=1,6)/0.334E+00,6
     2.250E+00,0.0E+00,10.77E+00,24.1E+00,24.1E+00/,ICODE/2/
C****
C**** TEST FOR WRITE CONTROL
C****
      IST = INDFA
      IPRINT = 0
      IF(MIX(IST+1).EQ.0.0) IPRINT = 1
C****
C**** SET PRESSURE LOOP
C****
      DO 8000 J = 1,NPT
C****
C**** CALCULATE CONCENTRATIONS
C****
      BCON1(J,IST) = CONCKI(1,J)
      BCON2(J,IST) = CONCKI(2,J)
      BCON6(J,IST) = CONCKI(6,J)
      DO 1000 I = 1,10
      CONMCM(I,J,IST) = (CONCKI(I,J)*PPP(J))/(82.057*TTT(J))
 1000 CONTINUE
C****
C**** COMPUTE RATE CONSTANTS
C****
      DO 2000 I =1,6
      RATEK(I,J,IST) = A(I)*(TTT(J)**EN(I))*EXP(-E(I)/(1.987E-03*TTT(J))
     1)
 2000 CONTINUE
C****
C**** CALCULATE FORWARD REACTION CONSTANTS
C****
      R1(J,IST) = (RATEK(1,J,IST)*CONMCM(5,J,IST)*CONMCM(6,J,IST))
      R2(J,IST) = (RATEK(2,J,IST)*CONMCM(5,J,IST)*CONMCM(9,J,IST))
      R3(J,IST) = (RATEK(3,J,IST)*CONMCM(5,J,IST)*CONMCM(10,J,IST))
      R4(J,IST) = (RATEK(4,J,IST)*CONMCM(4,J,IST)*CONMCM(7,J,IST))
      R5(J,IST) = (RATEK(5,J,IST)*CONMCM(8,J,IST)*CONMCM(7,J,IST))
      R6(J,IST) = (RATEK(6,J,IST)*CONMCM(8,J,IST)*CONMCM(7,J,IST))
C****
C**** CALCULATE K1,K2,RHO,KS, AND PHI
C****
      IF(R2(J,IST).EQ.0.0.AND.R3(J,IST).EQ.0.0) EK1(J,IST) = 1.0E+35
      IF(R2(J,IST).EQ.0.0.AND.R3(J,IST).EQ.0.0) GO TO 2500
      EK1(J,IST) = (R1(J,IST)/(R2(J,IST)+R3(J,IST)))
 2500 IF(R4(J,IST).EQ.0.0.AND.R5(J,IST).EQ.0.0) EK2(J,IST) = 1.0E+35
      IF(R4(J,IST).EQ.0.0.AND.R5(J,IST).EQ.0.0) GO TO 2750
      EK2(J,IST) = (R6(J,IST)/(R4(J,IST)+R5(J,IST)))
 2750 ROH(J,IST) = (PPP(J)*WM(J))/(82.057*TTT(J))
C****
```

```
C**** NOTE...FUEL CARD IS PHYSICALLY BEFORE OXIDANT CARD IN INPUT,OXYGEN
C**** IS SECOND SPECIE SPECIFIED IN OXIDANT AIR,FUEL IS SPECIFIED C-A,
C**** H-B
C****
      EKS = ((12.*ANUM(1,1)+1.*ANUM(1,2))*ANUM(2,2))/(28.99*(ANUM(1,1)+(
     1ANUM(1,2)/4.)))
      PHI(IST) =  RON/EKS
      F(IST) = PHI(IST)*EKS/(1.+(PHI(IST)*EKS))
C****
C**** CALCULATE CONCENTRATION OF CH2
C****
      RATWTS = ANUM(1,1)/ANUM(1,2)
      CH2(J,IST) = (((RATWTS/(1.+12.*RATWTS))*(WM(J)*RON/(RON+1.)))-CONC
     1KI(2,J)-CONCKI(3,J)-CONCKI(1,J))
C****
C**** STORE VALUES OF T
C****
      ATT(J,IST) = TTT(J)
 6000 CONTINUE
C****
C**** PRINT AND PUNCH OUTPUT
C****
      IF(IPRINT.EQ.0) GO TO 9999
      DO 9500 J = 1,NPT
      DO 9000 I =1,IST
      IF(I.NE.1) GO TO 8500
      WRITE(6,8100) ANUM(1,1),ANUM(1,2),RTEMP(2),PPP(J),ICODE,EKS
      WRITE(7,8100) ANUM(1,1),ANUM(1,2),RTEMP(2),PPP(J),ICODE,EKS
 8100 FORMAT(1X,7HFUEL= C,E15.8,1HH,E15.8,18H INLET AIR T.(K)= ,E15.8/1X
     1,13HPRESS.(ATM)= ,E15.8,7HICODE= ,I2,13HPHI STOICH.= ,E15.8)
 8500 WRITE(6,8200) F(I),PHI(I),ROH(J,I),ATT(J,I),BCON6(J,I),BCON2(J,I),
     1HCON1(J,I),CH2(J,I),R1(J,I),R6(J,I),EK1(J,I),EK2(J,I)
 8200 FORMAT(1X,6E12.5/1X,6E12.5)
      WRITE(7,8250) F(I),PHI(I),ROH(J,I),ATT(J,I),BCON6(J,I),BCON2(J,I),
     1HCON1(J,I),CH2(J,I),R1(J,I),R6(J,I),EK1(J,I),EK2(J,I)
 8250 FORMAT(6E12.5/6E12.5)
 9000 CONTINUE
 9500 CONTINUE
 9999 RETURN
      END
```

APPENDIX VI - LISTING OF PROGRAM NOXRAT

```
      PROGRAM NOXRAT(INPUT,OUTPUT,PUNCH,TAPE 5 = INPUT,TAPE 6 = OUTPUT,T
     1APE 7 = PUNCH,TAPE 4)
C
C  MAIN PROGRAM
C
      DOUBLE PRECISION G,X
      REAL MIX(50)
      INTEGER DATA, OMIT, ENSERT, REAC, BLANK, THRM, END,SUB
      LOGICAL HP,SP,TP,IDEBUG,NEWR,IONS,MOLES,FROZ,EQL,PSIA,RKT
      LOGICAL SHOCK,MMHG,PASCAL,EV,IC,DETN,CPCVFR,CPCVEQ,SIUNIT,EUNITS
      LOGICAL FA,OF,ERATIO,FPCT
C
      DIMENSION OMIT(3,3),NCO(4),ENSERT(3,3),LH(2),LVP(2) ,LVM(2)
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)
     2  ,TOTN(13)
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)
     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
     4 ,RHOP,RMW(15),TLN
      COMMON /DOUBLE/ G(20,21), X(20)
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,NLM
     1   ,NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK
      COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13)
     1 ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SS0
      COMMON/SNEW/RON,INDFA
      COMMON/DICK/MIX
      COMMON/EQNEW/R1(30,40),R6(30,40),EK1(30,40),EK2(30,40),ROH(30,40),
     1CH2(30,40),ATT(13,40),F(40),PHI(40),BCON1(30,40),BCON2(30,40),BCON
     26(30,40)
C
      EQUIVALENCE (OMIT,ENLN),(ENSERT,EN(1,3)),(NLM,L),(OF,OXFL)
C
      DATA MIT/4HOMIT/,BLANK/1H /, PSIA/4HPSIA/,REAC/4HREAC/,IZ/2H00/
     1   ,INPUT/4HINPU/,IE/1HE/,INSERT/4HINSE/,THRM/4HTHER/,END/3HEND/
      DATA LH/4HH,CA,4HL/G /,LVP/2HV+,1H /,LVM/2HV-,1H /,NMLT/4HNAME/
C
      NAMELIST/INPT2/KASE,P,T,ERATIO,OF,FPCT,FA,TP,HP,SP,RKT
     1,PSIA,MMHG,SHOCK,IONS,EV,V,DETN,CPCVFR,CPCVEQ,IDEBUG
     2,SIUNIT,EUNITS,MIX
C
      TLOW = 0.
      NEWR = .FALSE.
C
    1 WRITE(6,400)
  400 FORMAT(1H1)
  203 READ (5,204) (DATA(I),I=1,15)
  204 FORMAT(5(3A4,3X))
      WRITE (6,2045)(DATA(I),I=1,15)
 2045 FORMAT(1X,5(3A4,3X))
      IF(DATA(1).EQ.THRM)  GO TO 90
      IF(DATA(1).EQ.REAC)  GO TO 11
      IF (DATA(1).EQ.MIT) GO TO 205
      IF (DATA(1).EQ.INSERT) GO TO 180
      IF(DATA(1).EQ.INPUT.OR.DATA(1).EQ.NMLT)  GO TO 210
      IF(DATA(1).EQ.BLANK) GO TO 203
```

```
 1023 WRITE(6,1024)                                                      NOX*0600
 1024 FORMAT(40H0ERROR IN ABOVE CARD.  IGNORE CONTENTS.                  NOX*0610
      GO TO 203                                                          NOX*0620
   11 NOMIT = 0                                                          NOX*0630
      NSERT = 0                                                          NOX*0640
      MOLES = .FALSE.                                                    NOX*0650
      CALL REACT                                                         NOX*0660
      IF(L.EQ.0)  WRITE(6,52)                                            NOX*0670
   52 FORMAT(24H0ERROR IN REACTANT CARDS)                                NOX*0680
      GO TO 203                                                          NOX*0690
C                                                                        NOX*0700
C     READ THERMO DATA FROM CARDS AND STORE ON  TAPE 4                   NOX*0710
C                                                                        NOX*0720
   90 NEWR = .TRUE.                                                      NOX*0730
      REWIND 4                                                           NOX*0740
      READ(5,5) TLOW,TMID,THIGH                                          NOX*0750
    5 FORMAT (3F10.3)                                                    NOX*0760
      WRITE (4,5) TLOW,TMID,THIGH                                        NOX*0770
   97 READ (5,10)(DATA(I),I=1,16),NCD(1)                                 NOX*0780
   10 FORMAT(3A4,6X,2A3,4(A2,F3.0),A1,2F10.3,I15)                        NOX*0790
      IF(DATA(1).EQ.BLANK) DATA(1)=END                                   NOX*0800
      WRITE (4,10)(DATA(I),I=1,16)                                       NOX*0810
      IF(DATA(1).EQ.END)   GO TO 203                                     NOX*0820
      READ(5,20)(DATA(I),I=1,5),NCD(2),(DATA(J),J=6,10),NCD(3),(DATA(K), NOX*0830
     1K=11,14),NCD(4)                                                    NOX*0840
   20 FORMAT(5E15.8,I5/5E15.8,I5/4E15.8,I20)                             NOX*0850
      WRITE (4,21)(DATA(I),I=1,14)                                       NOX*0860
   21 FORMAT(5E15.8/5E15.8/4E15.8)                                       NOX*0870
      DO 25  I=1,4                                                       NOX*0880
      IF(NCD(I).EQ.I)   GO TO 25                                         NOX*0890
      WRITE(6,22)  (DATA(J),J=1,3)                                       NOX*0900
   22 FORMAT(28H0ERROR IN ORDER OF CARDS FOR ,3A4)                       NOX*0910
   25 CONTINUE                                                           NOX*0920
      GO TO 97                                                           NOX*0930
C                                                                        NOX*0940
C     CHECK INSERT CARDS                                                 NOX*0950
C                                                                        NOX*0960
  180 DO 185 I=4,15,3                                                    NOX*0970
      IF (DATA(I).EQ.BLANK) GO TO 185                                    NOX*0980
      NSERT = NSERT+1                                                    NOX*0990
      ENSERT(1,NSERT) = DATA(I)                                          NOX*1000
      ENSERT(2,NSERT) = DATA(I+1)                                        NOX*1010
      ENSERT(3,NSERT) = DATA(I+2)                                        NOX*1020
  185 CONTINUE                                                           NOX*1030
      GO TO 203                                                          NOX*1040
C                                                                        NOX*1050
C     CHECK OMIT CARDS                                                   NOX*1060
C                                                                        NOX*1070
  205 DO 208  I=4,15,3                                                   NOX*1080
      IF(DATA(I).EQ.BLANK) GO TO 208                                     NOX*1090
      NOMIT = NOMIT+1                                                    NOX*1100
      OMIT(1,NOMIT) = DATA(I)                                            NOX*1110
      OMIT(2,NOMIT) = DATA(I+1)                                          NOX*1120
      OMIT(3,NOMIT) = DATA(I+2)                                          NOX*1130
  208 CONTINUE                                                           NOX*1140
      NEWR= .TRUE.                                                       NOX*1150
      GO TO 203                                                          NOX*1160
C                                                                        NOX*1170
C     BEGIN NAMELIST INPT2                                               NOX*1180
C                                                                        NOX*1190
```

```
210 DO 300 I=1,26                                                       NOX*1200
    PCP(I) = 0.                                                         NOX*1210
    P(I)= 0.                                                            NOX*1220
    T(I)= 0.                                                            NOX*1230
    V(I) = 0.                                                           NOX*1240
300 CONTINUE                                                            NOX*1250
    V1 = 0.                                                             NOX*1260
    V2 = 0.                                                             NOX*1270
    RHOP = 0.                                                           NOX*1280
    KASE= 0                                                             NOX*1290
    TP = .FALSE.                                                        NOX*1300
    HP=.FALSE.                                                          NOX*1310
    SP=.FALSE.                                                          NOX*1320
    RKT = .FALSE.                                                       NOX*1330
    CPCVFR = .FALSE.                                                    NOX*1340
    CPCVEQ = .FALSE.                                                    NOX*1350
    SHOCK = .FALSE.                                                     NOX*1360
    DETN = .FALSE.                                                      NOX*1370
    EV = .FALSE.                                                        NOX*1380
    PASCAL = .FALSE.                                                    NOX*1390
    MMHG   = .FALSE.                                                    NOX*1400
    PSIA = .FALSE.                                                      NOX*1410
    R = 1.987165                                                        NOX*1420
    RR = 4184.*R                                                        NOX*1430
    SIUNIT = .FALSE.                                                    NOX*1440
    EUNITS = .FALSE.                                                    NOX*1450
    IONS = .FALSE.                                                      NOX*1460
    IDEBUG=.FALSE.                                                      NOX*1470
    FA= .FALSE.                                                         NOX*1480
    OF= .FALSE.                                                         NOX*1490
    ERATIO = .FALSE.                                                    NOX*1500
    FPCT= .FALSE.                                                       NOX*1510
    DO 303 I = 1,50                                                     NOX*1520
    MIX(I) = 0.                                                         NOX*1530
303 CONTINUE                                                            NOX*1540
    EQL = .TRUE.                                                        NOX*1550
    READ(5,INPT2)                                                       NOX*1560
    DO 305 I=1,26                                                       NOX*1570
    IF(P(I ).EQ.0.) GO TO 322                                           NOX*1580
    NP = I                                                              NOX*1590
    IF (MMHG) P(NP) = P(NP)/760.                                        NOX*1600
    IF (PASCAL) P(NP) = P(NP)/101325.                                   NOX*1610
    IF(PSIA           )  P(NP)=P(NP)/14.696006                          NOX*1620
305 CONTINUE                                                            NOX*1630
322 DO 625 IST =1,40                                                    NOX*1640
    INOFA = IST                                                         NOX*1650
    IF(IST.NE.1)  WRITE(6,400)                                          NOX*1660
    IF( MIX  (IST).NE.0.) GO TO 323                                     NOX*1670
    IF(IST.NE.1) GO TO 1                                                NOX*1680
    WRITE(6,724)                                                        NOX*1690
724 FORMAT(48HONO INPT2 VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT          NOX*1700
    IF (WP(2).NE.0.) OXFL = WP(1)/WP(2)                                 NOX*1710
    GO TO 333                                                           NOX*1720
323 OXFL  = MIX(IST)                                                    NOX*1730
    RON = MIX(IST)                                                      NOX*1740
    IF(FA) OXFL =1./   MIX(IST)                                         NOX*1750
    IF(FPCT) OXFL =(100.-   MIX(IST))/   MIX(IST)                       NOX*1760
    IF(.NOT.ERATIO)  GO TO 333                                          NOX*1770
    EQRAT = MIX(IST)                                                    NOX*1780
    IF(EQRAT.EQ.1.)  EQRAT = 1.000005                                   NOX*1790
```

```
      OXFL   = (-EQRAT*VMIN(2)-VPLS(2))/(VPLS(1)+EQRAT*VMIN(1))
  333 SUM = OXFL +1.
      V2 = (OXFL*VMIN(1)+VMIN(2))/SUM
      V1 = (OXFL*VPLS(1)+VPLS(2))/SUM
      IF(V2.NE.0.)  EQRAT=ABS(V1/V2)
      IF (RHO(1) .NE. 0. .AND. RHO(2) .NE. 0.) GO TO 744
      RHOP = RHO(2)
      IF (RHOP .EQ. 0.) RHOP = RHO(1)
      GO TO 745
  744 RHOP =(OXFL+1.)*RHO(1)*RHO(2)/(RHO(1)+OXFL*RHO(2))
  745 LL = L
      IF (.NOT.IONS) GO TO 746
      LL = L-1
      IF (LLMT(L).EQ.IE) GO TO 746
      LL = L
      L = L+1
      LLMT(L) = IE
      BO(L) = 0.
  746 DO 747 I=1,LL
      BO(I) = (OXFL *BOP(I,1)+      BOP(I,2))/SUM
  747 CONTINUE
      NPT = 1
      HSUB0=(OXFL*HPP(1) + HPP(2))/SUM
      IF (.NOT.NEWR) GO TO 786
      CALL SEARCH
      IF(SHOCK.OR.DETN)  GO TO 760
      DO 755 N=1,NREAC
      IF(NAME(N,5).NE.IZ)  GO TO 755
      TT = RTEMP(N)
      CALL HCALC
      GO TO 760
  755 CONTINUE
  760 WRITE(6,INPT2)
  786 ENN = .1
      SUMN = ENN
      XI = NS - NC
      XI = ENN/XI
      XLN = ALOG(XI)
      DO 432 J=1,NS
      IF(IUSE(J).EQ.-10000)  IUSE(J)=0
      IF (IUSE(J).NE.0)  GO TO 432
      EN(J,1) = XI
      ENLN(J) = XLN
  432 CONTINUE
      WRITE (6,770)
  770 FORMAT (1H0,17X,4HFUEL ,13X,7HOXIDANT  ,12X,7HMIXTURE   //)
  780 FORMAT (1H 2A4,3E18.8/)
      WRITE (6,780) LH,HPP(2),HPP(1),HSUB0,LVP,VPLS(2),VPLS(1),V1,
     1LVM,VMIN(2),VMIN(1),V2
      HSUB0 = HSUB0/R
      WRITE (6,785)
  785 FORMAT (8H ATOMS/G   )
      WRITE(6,780)(LLMT(I),BLANK,BOP(I,2),BOP(I,1),BO(I),I=1,L)
      IQ1= L+1
      IF(NC.EQ.0)  GO TO 790
      DO 302 J=1,NS
      IF(IUSE(J).EQ.0) GO TO 302
      IF(IUSE(J).GT.0) IUSE(J)= -IUSE(J)
      EN(J,1) = 0.
      ENLN(J)=0.
```

```
      IF(NSERT.EQ.0) GO TO 302
      DO 301 I=1,NSERT
      IF(SUB(J,1).NE.ENSERT(1,I)) GO TO 301
      IF(SUB(J,2).NE.ENSERT(2,I)) GO TO 301
      IF(SUB(J,3).NE.ENSERT(3,I)) GO TO 301
      ENSERT(1,I) =0.
      IQ1= IQ1+1
      IUSE(J)= -IUSE(J)
  301 CONTINUE
  302 CONTINUE
  790 ITN= 35
      IC = .FALSE.
      JSOL = 0
      JLIQ = 0
      IF(DETN) CALL DETON
      IF(RKT) CALL ROCKET
      IF (TP) CALL MOLIER
      IF(HP) CALL CMBSTN
      IF(SHOCK)  CALL SHCK
  625 CONTINUE
      NSERT = 0
      GO TO 1
      END
```

```
      SUBROUTINE REACT
C
      DOUBLE PRECISION G,X
      LOGICAL HP,SP,TP,IDEBUG,CONVG,NEWR,IONS,MOLES,EQL,FROZ
C
      DIMENSION ANAME(15,5),V(15)
C
      COMMON/MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
     4 ,RHOP,RMW(15),TLN
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,NLM
     1  ,NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK
C
      EQUIVALENCE (NAME,ANAME),(NLM,L)
C
      DATA MOL/1HM/,OX/1HO/,LANK/1H /,IZERO/2H00/
C
      DO 10 K=1,2
      WP(K)=0.
      HPP(K)=0.
      RHO(K)=0.
      VPLS(K)=0.
      VMIN(K)=0.
      AC(K)=0.
      AM(K)=0.
      DO 8 J=1,15
      LLMT(J)=0
      B0P(J,K)=0.
    8 CONTINUE
   10 CONTINUE
      N=1
      L=1
   20 READ(5,21) (NAME(N,I),ANUM(N,I),I=1,5),PECWT(N),MOLE,ENTH(N),FAZ(N)
     1 ,RTEMP(N),FOX(N),DENS(N)
   21 FORMAT(5(A2,F7.5),F7.5,A1,F9.5,A1,F8.5,A1,F8.5)
      IF(NAME(N,1).EQ.LANK) GO TO 200
      IF(L.EQ.0)GO TO 20
      WRITE (6,31) (NAME(N,I),ANUM(N,I),I=1,5),PECWT(N),MOLE,ENTH(N),FAZ
     1 (N),RTEMP(N),FOX(N),DENS(N)
   31 FORMAT(1X,5(A2,1X,F7.4,2X),F8.4,2X,A1,F11.2,2X,A1,2X,F8.3,2X,
     1A1,3X,F8.5)
   35 IF(MOLE.EQ.MOL) MOLES=.TRUE.
      K=2
      IF(FOX(N).EQ.OX)K=1
      DO 38 J=1,15
      DATA(J) = 0.
   38 CONTINUE
      RM=0.
      DO 100 JJ=1,5
      IF(ANUM(N,JJ).EQ.0.)GO TO 101
      DO 41 J=1,15
      NJ = J
      IF(LLMT(J).EQ.0) GO TO 45
      IF(NAME(N,JJ).EQ.LLMT(J))GO TO 46
   41 CONTINUE
   45 L = NJ
      LLMT(J)=NAME(N,JJ)
```

```
 46 DO 48 KK=1,101
    IF(ATOM(1,KK).EQ.ANAME(N,JJ))GO TO 50
 48 CONTINUE
    L=0
    GO TO 20
 50 RM=RM+ANUM(N,JJ)*ATOM(2,KK)
    V(J)=ATOM(3,KK)
    DATA(J)=ANUM(N,JJ)
100 CONTINUE
101 PCWT=PECWT(N)
    IF(MOLES) PCWT=PCWT*RM
    WP(K)=WP(K) + PCWT
    IF(NAME(N,5).NE.IZERO)HPP(K)=HPP(K)+ENTH(N)*PCWT/RM
    AM(K)=AM(K)+PCWT/RM
    DO 110  J=1,L
    BOP(J,K)=DATA(J)*PCWT/RM +BOP(J,K)
110 CONTINUE
    IF(DENS(N).NE.0.)GO TO 115
    GO TO 117
115 RHO(K)=RHO(K)+PCWT/DENS(N)
117 RMW(N) = RM
    N = N+1
    IF(N.NE.16) GO TO 20
200 NREAC =N-1
    IF(L.EQ.0) GO TO 1000
    DO 220 K=1,2
    IF(WP(K).EQ.0.)GO TO 220
    HPP(K)=HPP(K)/WP(K)
    AM(K) = WP(K)/AM(K)
    IF(RHO(K).NE.0.)RHO(K)=WP(K)/RHO(K)
    DO 215 J=1,L
    BOP(J,K)=BOP(J,K)/WP(K)
    IF(V(J).LT.0.)VMIN(K)= VMIN(K)+BOP(J,K)*V(J)
    IF(V(J).GT.0.)VPLS(K)=VPLS(K)+BOP(J,K)*V(J)
215 CONTINUE
    IF(MOLES) GO TO 220
    DO 218 N=1,NREAC
    IF(FOX(N).EQ.OX.AND.K.EQ.2)  GO TO 218
    IF(FOX(N).NE.OX.AND.K.EQ.1)  GO TO 218
    PECWT(N) = PECWT(N)/WP(K)
218 CONTINUE
220 CONTINUE
    NEWR=.TRUE.
    DO 230 N = 1,NREAC
    IF (DENS(N).NE.0.) GO TO 230
    RHO (1) = 0.
    RHO(2) = 0.
    GO TO 1000
230 CONTINUE
1000 RETURN
    END
```

```
      SUBROUTINE SEARCH
C
C  SEARCH TAPE FOR THERMO DATA FOR SPECIES TO BE CONSIDERED
      INTEGER SUB,OMIT,END
C
      LOGICAL NEWR
C
      DIMENSION DATE(2,3),MT(4),B(4),OMIT(3,3)
C
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)
     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
     4 ,RHOP,RMW(15),TLN
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,NLM
     1  ,NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK
C
      EQUIVALENCE (DATE,EN),(OMIT,ENLN),(ENDD,END),(L,NLM)
C
      DATA  GAS/1HG/,END/3HEND/
C
      NC= 0
      IX= 0
      COEF(1,1,1) = ENDD
      I = I
      DO 3 I=1,150
      IF(A(1,I).EQ.ENDD)  GO TO 4
      DO 3  J=1,L
      A(J,I) = 0.
    3 CONTINUE
    4 MAXNS = I
      REWIND 4
      READ(4,5)  TLOW,TMID,THIGH
    5 FORMAT (3F10.3)
      NS = 1
    7 READ      (4,10)(SUB(NS,I),I=1,3),DATE(1,NS),DATE(2,NS),(MT(J),B(J),
     1  J=1,4),PHAZ,T1,T2
   10 FORMAT(3A4,6X,2A3,4(A2,F3.0),A1,2F10.3)
      IF(SUB(NS,1).EQ.END) GO TO 171
      READ      (4,20)  ((COEF(I,J,NS),J=1,7),I=1,2)
   20 FORMAT (5E15.8)
      IF(NOMIT.EQ.0) GO TO 810
      DO 805 I=1,NOMIT
      DO 804 J=1,3
      IF(OMIT(J,I).NE.SUB(NS,J)) GO TO 805
  804 CONTINUE
      GO TO 7
  805 CONTINUE
  810 DO 820 K=1,4
      IF(B(K).EQ.0.) GO TO 825
      DO 168 I=1,L
      IF(LLMT(I).EQ.MT(K)) GO TO 820
  168 CONTINUE
      DO 819 J=1,L
  819 A(J,NS) = 0.
      GO TO 7
  820 A(I,NS)= B(K)
```

```
825 IF(NS.EQ.MAXNS)  GO TO 870                                          SEA*0600
    IUSE(NS)= 0                                                         SEA*0610
    IF(PHAZ.EQ.GAS) GO TO 170                                           SEA*0620
    NC= NC+1                                                            SEA*0630
    TEMP(NC,1)= T1                                                      SEA*0640
    TEMP(NC,2)= T2                                                      SEA*0650
    IX= IX+1                                                            SEA*0660
    IF(IUSE(NS-1).EQ.0 .OR. NC.EQ.1) GO TO 145                          SEA*0670
    DO 830 I=1,L                                                        SEA*0680
    IF(A(I,NS).NE.A(I,NS-1)) GO TO 145                                  SEA*0690
830 CONTINUE                                                            SEA*0700
    IX= IX-1                                                            SEA*0710
145 IUSE(NS)= -IX                                                       SEA*0720
170 NS= NS+1                                                            SEA*0730
    GO TO 7                                                             SEA*0740
870 WRITE(6,871) (SUB(NS,J),J=1,3)                                      SEA*0750
871 FORMAT (45H0DIMENSIONS IN/SPECES/TOO SHALL TO CONSIDER ,3A4)        SEA*0760
    GO TO 7                                                             SEA*0770
171 NS= NS-1                                                            SEA*0780
    NEWR= .FALSE.                                                       SEA*0790
    WRITE(6,172)                                                        SEA*0800
172 FORMAT(42H0SPECIES BEING CONSIDERED IN THIS SYSTEM                  SEA*0810
    DO 174 I=1,NS,5                                                     SEA*0820
    I5= I+4                                                             SEA*0830
    IF(NS.LT.I5) I5=NS                                                  SEA*0840
174 WRITE (6,176)(DATE(1,J),DATE(2,J),SUB(J,1),SUB(J,2),SUB(J,3),J=I,   SEA*0850
   1  I5)                                                               SEA*0860
176 FORMAT(5(5X,2A3,2X,3A4))                                            SEA*0870
    RETURN                                                              SEA*0880
    END                                                                 SEA*0890
```

```
      SUBROUTINE EQLBRM
C  ROUTINE TO CALCULATE EQUILIBRIUM COMPOSITION AND PROPERTIES
C
      DOUBLE PRECISION X,G
      LOGICAL HP,SP,TP,IDEBUG,CONVG,IONS,MOLES,FROZ,EQL,LOGV,HPSP,TPSP
      LOGICAL ISING,IC,SHOCK
C
      DIMENSION PROW(18)
C
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)
     2,TOTN(13)
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)
     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
     4 ,RHOP,RMW(15),TLN
      COMMON /DOUBLE/ G(20,21), X(20)
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,NLM
     1   ,NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK
      COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13)
     1 ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SS0
C
      EQUIVALENCE (NLM,L)
C
      DATA               IE/1HE/,SMALNO/1.E-6/,SMNOL/-13.815511/
C
      SIZE= 18.5
      SIZEF = 0.
      ISING = .FALSE.
      ENNL = ALOG(ENN)
      LOGV = .FALSE.
      PPLN = ALOG(PP)
      TLN = ALOG(TT)
      CONVG = .FALSE.
      ITNUMB = ITN
      JS1 = 1
      CALL CPHS
      TM = PPLN - ENNL
C
C     IF(IC) PREVIOUS POINT HAD SINGULAR MATRIX
C
      IF(IC)  GO TO 966
      IF (.NOT.IONS.OR.IE.EQ.LLMT(L)) GO TO 33
      L = L+1
      IQ1 = IQ1+1
      DO 499 J = 1,NS
      IF (A(L,J) .EQ.0.) GO TO 499
      EN(J,NPT) = SMALNO
      ENLN(J) = SMNOL
      IUSE(J) = 0
  499 CONTINUE
   33 IF(NPT.EQ.1.AND..NOT.SHOCK)         WRITE(6,244) (LLMT(I),I=1,L)
  244 FORMAT (4H0PT ,14(5X,A4))
C
C     BEGIN ITERATION
C
```

```
   43 CONTINUE
      IF(IC)  GO TO 1171
      IF (.NOT.CONVG.OR.JSOL.EQ.0)  GO TO 62
      ENSOL = EN(JSOL,NPT)
      EN(JSOL,NPT) = EN(JSOL,NPT)+EN(JLIQ,NPT)
      IUSE(JLIQ) = -IUSE(JLIQ)
      IQ1 = IQ1-1
      DLVTP(NPT) = 0.
      CPR(NPT) = 0.
      GAMMAS(NPT) = 0.
      LOGV = .TRUE.
   62 CALL MATRIX
      NUMB = ITN-ITNUMB+1
      IF(.NOT.CONVG)    GO TO 67
      IF (LOGV.AND.JSOL.EQ.0) GO TO 63
      DO 182  I=1,L
      PROW(I) = G(IQ1,I)
  182 CONTINUE
      IF (.NOT.LOGV) GO TO 67
C
C     LOGV = .TRUE.-- SET UP MATRIX TO SOLVE FOR DLVPT
C
   63 G(IQ1,IQ2) = ENN
      IQ = IQ1 - 1
      DO 777 I = 1,IQ
      G(I,IQ2) = G(I,IQ1)
  777 CONTINUE
   67 IF (.NOT.IDEBUG) GO TO 72
      WRITE(6,772) NUMB
  772 FORMAT (11H0ITERATION  ,I3,6X,7HMATRIX //)
      DO 911 I=1,IMAT
  911 WRITE (6,73) (G(I,K),K=1,KMAT)
   72 IF(CONVG)  IMAT=IMAT-1
      ITST = IMAT
      CALL MGAUSD
      IF(ITST.NE.IMAT)  GO TO 774
      IF(.NOT.IDEBUG.OR.CONVG)  GO TO 773
      WRITE (6,373)(LLMT(I),I=1,L)
  373 FORMAT (7H0PI      ,9(A4,10X))
      WRITE (6,73)(X(I),I=1,IMAT)
   73 FORMAT (9F14.6)
  773 IF(.NOT.CONVG)  GO TO 85
      IF(.NOT.LOGV)  GO TO 174
      IF(JLIQ.NE.0) EN(JSOL,NPT)=ENSOL
      GO TO 171
  174 SUM = 0.
      DO 175 J=1,L
      SUM = SUM+PROW(J)*X(J)
  175 CONTINUE
      DLVTP(NPT) = 1.+G(IQ2,IQ1)/ENN-SUM/ENN  - X(IQ1)
      CPR(NPT) = G(IQ2,IQ2)
      DO 176 J=1,IQ1
      CPR(NPT) = CPR(NPT)-G(IQ2,J)*X(J)
  176 CONTINUE
      LOGV = .TRUE.
      GO TO 62
C
C  SINGULAR MATRIX
C
C     IF(ISING)  SINGULAR ONCE
```

```
C     IF(IC)      SINGULAR TWICE
C
  774 IF(.NOT.CONVG)  GO TO 775
      WRITE(6,172)
  172 FORMAT(28H0DERIVATIVE MATRIX SINGULAR )
      IC = .TRUE.
      GO TO 1171
  775 IF (.NOT.HP.OR.NPT.NE.1.OR.NC.EQ.0.OR.TT.GT.100.)  GO TO 871
      WRITE(6,874)
  874 FORMAT(96H0LOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE
     1BEEN INCLUDED ON AN INSERT CARD, RESTART )
      GO TO 873
  871 WRITE (6,74)
   74 FORMAT(16H0SINGULAR MATRIX)
      IF(IC)  GO TO 873
      IF (ISING) GO TO 997
      NTZERO = 0
  966 DO 970 JJ = 1, NS
      IF(IUSE(JJ)) 970,968,967
  967 IF(EN(JJ,NPT).EQ.0.)  GO TO 873
      GO TO 969
  968 IF(EN(JJ,NPT).NE.0.)  GO TO 969
      EN(JJ,NPT) = SMALNO
      ENLN(JJ) = SMNOL
      GO TO 970
  969 NTZERO = NTZERO+1
  970 CONTINUE
      IF(.NOT.IC)  GO TO 971
      IC = .FALSE.
      GO TO 43
  971 ISING = .TRUE.
      WRITE (6,776)
  776 FORMAT (8H0RESTART)
      GO TO 43
  997 IF(NTZERO.NE.(L-1))  GO TO 873
      IF(EQRAT.GT.1.00001.OR.EQRAT.LT.0.99999) GO TO 873
      ENN=0.
      NEN = 0
      DO 83  I=1,L
      JEN=0
      DO 80  J=1,NS
      IF(EN(J,NPT).EQ.0.)  GO TO 80
      IF(A(I,J).EQ.0.)  GO TO 80
      IF(JEN.NE.0)  GO TO 83
      JEN = J
   80 CONTINUE
      NEN = NEN+1
      EN(JEN,NPT) = B0(I)/A(I,JEN)
   83 CONTINUE
      IF(NEN.LT.NTZERO)  GO TO 873
      CONVG = .TRUE.
      IC = .TRUE.
      HSUM(NPT) = 0.
      DO 84  J=1,NS
      IF(EN(J,NPT).EQ.0.)  GO TO 84
      ENN = EN(J,NPT)+ENN
      TEM = EN(J,NPT)
      ENLN(J) = ALOG(TEM)
      HSUM(NPT) = HSUM(NPT) + EN(J,NPT)*H0(J)
   84 CONTINUE
```

```
      TM = ALOG(PP/ENN)
      GO TO 43
   85 ITNUMB= ITNUMB-1
C
C     OBTAIN CORRECTIONS TO THE ESTIMATES
C
      KK = L + 1
      DLNT= X(IQ2)
      IF (TP) DLNT=0.
      DO 101 J=1,NS
      IF (IUSE(J)) 101,98,100
   98 DELN(J) = H0(J)*DLNT-H0(J)+S(J)-ENLN(J)-TM+X(IQ1)
      DO 99 K=1,L
      DELN(J)= DELN(J)+A(K,J)*X(K)
   99 CONTINUE
      GO TO 101
  100 DELN(J) = X(KK)
      KK = KK + 1
  101 CONTINUE
      AMBDA= 1.
      AMBDA1= 1.
      SUM = X(IQ1)
      IF(SUM.LT.0.)  SUM=-SUM
      IF(DLNT.GT.SUM)  SUM=DLNT
      IF(-DLNT.GT.SUM)  SUM=-DLNT
      DO 917 J=1,NS
      IF (IUSE(J).NE.0) GO TO 917
      IF((EN(J,NPT).GT.0.).AND.DELN(J).GT.SUM) SUM = DELN(J)
      IF((EN(J,NPT).NE.0.) .OR. DELN(J).LE.0.) GO TO 917
      SUM1 = (-9.212-ENLN(J)+ENNL)/(DELN(J)-X(IQ1))
      IF(SUM1.LT.0.)  SUM1=-SUM1
      IF (SUM1.LT.AMBDA1) AMBDA1 = SUM1
  917 CONTINUE
      IF(SUM.GT.2.)AMBDA=2./SUM
      IF (AMBDA1.LT.AMBDA) AMBDA = AMBDA1
      IF (.NOT.IDEBUG) GO TO 111
      WRITE(6,923) TT,ENN,ENNL,PP,PPLN,AMBDA
  923 FORMAT (3H0T=,E15.8,6H  ENN=,E15.8,7H  ENNL=E15.8,5H  PP=,E15.8,
     1 7H  PPLN=E15.8,8H  AMBDA=E15.8 )
      WRITE (6,924)
  924 FORMAT(1H0,18X,2HNI,12X,5HLN NI,8X,9HDEL LN NI,10X,4HH/RT,9X,4HS0/
     1R,12X,6H-G0/RT,9X,5H-G/RT  )
      DO 926 J=1,NS
      FNEG1 = S(J)-H0(J)
      FNEG2 = FNEG1
      IF(IUSE(J).EQ.0)  FNEG2=FNEG2-ENLN(J)-TM
      WRITE (6,925) SUB(J,1),SUB(J,2),
     1SUB(J,3),EN(J,NPT),ENLN(J),DELN(J),H0(J),S(J),FNEG1,FNEG2
  925 FORMAT (1X,3A4,7E15.6)
  926 CONTINUE
      WRITE (6,110)
  110 FORMAT(1H0)
C
C     APPLY CORRECTIONS TO ESTIMATES
C
  111 SUM = 0.
      ENNL = ENNL+AMBDA*X(IQ1)
      ENN = EXP(ENNL)
      TM = PPLN - ENNL
      DO 113 J=1,NS
```

```
      IF (IUSE(J)) 113,112,114
  112 ENLN(J)=ENLN(J)+AMBDA*DELN(J)
      EN(J,NPT) = 0.
      IF((ENLN(J)-ENNL+SIZE).LE.0.)  GO TO 113
      EN(J,NPT) = EXP(ENLN(J))
      SUM = SUM+EN(J,NPT)
      GO TO 113
  114 EN(J,NPT) = EN(J,NPT) + AMBDA * DELN(J)
  113 CONTINUE
      SUMN = SUM
      IF (TP) GO TO 115
      TLN= TLN+AMBDA*DLNT
      TT     = EXP(TLN)
      JS1 = 1
      CALL CPHS
  115 IF (LLMT(L).NE.IE) GO TO 116
C
C     CHECK ON REMOVING IONS
C
      DO 1116 J = 1,NS
      IF (A(L,J).EQ.0.) GO TO 1116
      IF (EN(J,NPT).GT.0.) GO TO 116
 1116 CONTINUE
      DO 1118  J=1,NS
      IF(A(L,J).NE.0.) IUSE(J) = -10000
 1118 CONTINUE
      L = L-1
      IQ1 = IQ1-1
      GO TO 43
C
C     TEST FOR CONVERGENCE
C
  116 IF (ITNUMB.EQ.0) GO TO 13
      IF (AMBDA.LT.1.) GO TO 43
      SUM = (ENN-SUMN)/ENN
      IF (SUM.LT.0.) SUM = -SUM
      IF (SUM.GT.0.5E-5) GO TO 43
      DO 130 J=1,NS
      IF (IUSE(J).LT.0) GO TO 130
      AA= DELN(J)/SUMN
      IF(AA.LT.0.)  AA=-AA
      IF (IUSE(J).EQ.0) AA = AA*EN(J,NPT)
  129 IF(AA.GT.0.5E-5)  GO TO 43
  130 CONTINUE
C
C     CALCULATE ENTROPY, CHECK ON DELTA S FOR SP PROBLEMS
C
      SSUM(NPT) = 0.
      DO 183 J=1,NS
      IF (NPT.EQ.1) SS0 = SS0 + EN(J,1)*S(J)
      SS = S(J)
      IF(IUSE(J).EQ.0)  SS=SS-ENLN(J)-TM
      SSUM(NPT) = SSUM(NPT)+SS*EN(J,NPT)
  183 CONTINUE
      IF(.NOT.SP.OR.NPT.EQ.1)  GO TO 13
      SS = SSUM(NPT) -S0
      IF(SS.LT.(-0.00005).OR.SS.GT.0.00005)  GO TO 43
      IF(IDEBUG)  WRITE(6,1183) SS
 1183 FORMAT(12H0DELTA S/R =,E15.8)
   13 CONVG= .TRUE.
```

```
      IF(TT    .LT.TLOW.OR.TT    .GT.THIGH)WRITE (6,306)TT    ,NPT
  306 FORMAT(17H0THE TEMPERATURE=E12.4,26H IS OUT OF RANGE FOR POINT,I5)
      IF(ITNUMB.NE.0) GO TO 160
      WRITE(6,973) ITN,NPT
  973 FORMAT(1HL,I2,69H ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREME
     1NTS FOR THE POINT        I5)
      IF (.NOT.HP.OR.NPT.NE.1.OR.NC.EQ.0.OR.TT.GT.100.)  GO TO 873
      WRITE(6,874)
      TT = T(1)
      RETURN
C
C     CONVERGENCE TESTS ARE SATISFIED, TEST CONDENSED SPECIES.
C
  160 IF(NC.EQ.0) GO TO 143
      SIZEF = 0.
      INC = 0
      DO 170 J = 1,NS
      IF (IUSE(J).EQ.0 .OR. IUSE(J).EQ.-10000) GO TO 170
      INC = INC + 1
      IF(IDEBUG) WRITE(6,144)(SUB(J,I),I=1,3),TEMP(INC,1),TEMP(INC,2),
     1IUSE(J),EN(J,NPT)
  144 FORMAT (1H0,3A4,2F10.3,3X,5HIUSE=,I4,E15.7)
      IF (EN(J,NPT))  146,148,169
  146 IF (J.NE.JSOL .AND. J .NE.JLIQ) GO TO 147
      JSOL = 0
      JLIQ = 0
  147 IQ1 = IQ1 - 1
      EN(J,NPT) = 0.
      GO TO 166
  148 KG = 1
      IF(IUSE(J).EQ.-IUSE(J+1)) GO TO 154
  151 IF(J.EQ.1.OR.IUSE(J).NE.-IUSE(J-1)) GO TO 153
      KG = -1
  154 JKG = J + KG
      IF (EN(JKG,NPT).LT.0.) GO TO 170
      TMELT = TEMP(INC,1)
      IMP = INC + KG
      IF(TMELT.EQ.TEMP(IMP,2  )) GO TO 158
      TMELT = TEMP(INC,2)
      IF (TMELT.EQ.TEMP(IMP,1)) GO TO 157
      WRITE (6,156)
  156 FORMAT (50H03 PHASES OF A CONDENSED SPECIES ARE OUT OF ORDER   )
C
C  JTH SPECIES A SOLID (EN=0), (J+KG)TH SPECIES A LIQUID (EN IS +
C
  157 IF(TT.GT.TMELT) GO TO 169
      IF (TP.AND.TT.EQ.TMELT) GO TO 169
      IF (TP)  GO TO 1165
      IF (TT.LE.TMELT-150.) GO TO 1165
      JSOL = J
      JLIQ = JKG
      GO TO 159
C
C  JTH SPECIES A LIQUID(EN=0), (J+KG)TH SPECIES A SOLID (EN IS +)
C
  158 IF (TT.LT.TMELT) GO TO 169
      IF (TP.AND.TT.EQ.TMELT) GO TO 169
      IF (TP)  GO TO 1165
      IF (TT.GE.TMELT+150.) GO TO 1165
      JSOL = JKG
```

```
      JLIQ = J
  159 TLN = ALOG (TMELT)
      TT = TMELT
      EN(JKG,NPT) = .5 * EN(JKG,NPT)
      EN(J,NPT) = EN(JKG,NPT)
      GO TO 165
C
C  WRONG PHASE INCLUDED FOR T INTERVAL, SWITCH EN
C
 1165 EN(J,NPT) = EN (JKG, NPT)
      IUSE(J) = -IUSE(J)
      IUSE (JKG) = -IUSE(JKG)
      EN(JKG,NPT)= 0.
      GO TO 40
  153 IF (TT.LT.TEMP(INC,1) .AND.TEMP(INC,1).NE.TLOW) GO TO 169
      IF (TT.GT.TEMP(INC,2)) GO TO 169
C
C
      SUM = 0.
      DO 167 I = 1,L
      SUM = SUM + A(I,J)*X(I)
  167 CONTINUE
      DELF = H0(J)-S(J)-SUM
      IF(IDEBUG) WRITE(6,168)DELF,SIZEF
  168 FORMAT (17H G0-SUM(AIJ*PI) =E15.7,10X,18HPREVIOUS DELTA G =,E15.7)
      IF(DELF.GE.SIZEF .OR. DELF.GE.0.) GO TO 169
      SIZEF = DELF
      JDELF = J
  169 IF(INC.EQ.NC) GO TO 1160
  170 CONTINUE
 1160 IF (SIZEF.EQ.0.) GO TO 143
      J = JDELF
  165 IQ1 = IQ1 + 1
  166 IUSE(J) = - IUSE(J)
   40 CONVG = .FALSE.
      IF(NPT.EQ.1)  SS0 =0.
      JS1 = 1
      CALL CPHS
  143 TN = NUMB
      IF(.NOT.SHOCK)          WRITE(6,771)NPT,(X(IL),IL=1,L),TN
  771 FORMAT (I3,14F9.3)
      ITNUMB = ITN
      JS1 = 1
      IF(TP.AND.CONVG)  CALL CPHS
      GO TO 43
C
C     CALCULATE EQUILIBRIUM PROPERTIES
C
 1171 DLVPT(NPT) = -1.
      DLVTP(NPT) = 1.
      CPR(NPT) = CPSUM
      GO TO 199
  171 SUM = 0.
      DO 179 J = 1,L
      SUM = SUM + PROW(J)*X(J)
  179 CONTINUE
      DLVPT(NPT) = -2.+SUM/ENN+ X(IQ1)
  184 IF(JLIQ.EQ.0)  GO TO 199
      IUSE(JLIQ) = -IUSE(JLIQ)
      HSUM(NPT) = HSUM(NPT)+EN(JLIQ,NPT)*(H0(JLIQ)-H0(JSOL))
```

```
      IQ1 = IQ1+1
      GAMMAS(NPT) = -1./DLVPT(NPT)
      GO TO 186
  199 GAMMAS(NPT) = -1./(DLVPT(NPT)+(DLVTP(NPT)**2)*ENN/CPR(NPT))
  186 TTT(NPT) = TT
      PPP(NPT) = PP
      CPRF(NPT) = CPSUM
      HSUM(NPT) = HSUM(NPT)*TT
      WM(NPT) = 1./ENN
  200 IF (.NOT.IDEBUG) RETURN
      PRATIO = 1.
      IF(SP)  PRATIO=PP/P(1)
      WRITE(6,201) NPT,PRATIO,  PP,TT,HSUM(NPT),SSUM(NPT),WM(NPT),CPR(NP
     1T),DLVPT(NPT),DLVTP(NPT),GAMMAS(NPT)
  201 FORMAT (7H0POINT=I3,3X,4HPCP=E13.6,3X,2HP=E13.6,3X,2HT=E13.6,3X,4H
     1H/R=E13.6,3X,4HS/R=E13.6//3X,3HMW=E13.6,3X,5HCP/R=E13.6,3X,6HDLVPT
     2=E13.6,3X,6HDLVTP=E13.6,3X,9HGAMMA(S)=E13.6 )
      GO TO 1000
C
C     ERROR. SET TT=0
C
  873 TT=0.
      NPT = NPT-1
 1000 RETURN
      END
```

```
      SUBROUTINE CPHS
C     CALCULATES THERMODYNAMIC PROPERTIES FOR INDIVIDUAL SPECIES
C
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)
     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
     4 ,RHOP,RMW(15),TLN
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,NLM
     1   ,NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK
C
      EQUIVALENCE (J,JS1)
C
      K = 1
      IF(TT.LE.TMID)K = 2
      KK = 0
      CPSUM=0.
   90 IF(COEF(K,1,J).NE.0.)GO TO 97
      IF (IUSE(J).LT.0) GO TO 100
      KK = K
      K = 1
      IF (KK.EQ.1) K = 2
   97 S(J) =   ((((COEF(K,5,J)/4.)*TT+ COEF(K,4,J)/3.)*TT+ COEF(K,3,J)/2.
     1)* TT+COEF(K,2,J))*TT+ COEF(K,1,J)*TLN + COEF(K,7,J)
      H0(J) = ((((COEF(K,5,J)/5.)*TT+ COEF(K,4,J)/4.)*TT+ COEF(K,3,J)/3.
     1  ) *TT+ COEF(K,2,J)/2.)*TT+ COEF(K,1,J) + COEF(K,6,J)/TT
      CPSUM= CPSUM+((((COEF(K,5,J)*TT+ COEF(K,4,J))*TT+ COEF(K,3,J))*TT
     1    + COEF(K,2,J))*TT+ COEF(K,1,J))*EN(J,NPT)
      IF (KK.EQ.0) GO TO 100
      K = KK
      KK = 0
  100 IF(J.EQ.NS) GO TO 200
      J=J+1
      GO TO 90
  200 RETURN
      END
```

```
      SUBROUTINE MATRIX
C
C
      DOUBLE PRECISION G,X
      LOGICAL HP,SP,TP,IDEBUG,CONVG,NEWR
C
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)
     2,TOTN(13)
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)
     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
     4 ,RHOP,RMW(15),TLN
      COMMON /DOUBLE/ G(20,21), X(20)
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TSP,MOLES,NP,NT,NPT,NLM
     1   ,NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFH,CPCVEQ
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK
C
      EQUIVALENCE (L,NLM)
C
      IQ2 = IQ1 + 1
      IQ3 = IQ2 + 1
      KMAT = IQ3
      IF(.NOT.CONVG.AND.TP) KMAT = IQ2
      IMAT = KMAT - 1
C
C     CLEAR MATRIX STORAGES TO ZERO
C
      DO 211 I=1,IMAT
      DO 211 K=1,KMAT
      G(I,K)= 0.0D0
  211 CONTINUE
      SSS = 0.
      HSUM(NPT) = 0.
C
C     BEGIN SET UP OF ITERATION MATRIX
C
      KK = L
      DO 65  J=1,NS
      H=H0(J)*EN(J,NPT)
      IF (IUSE(J)) 65,11,70
   11 F = (H0(J)-S(J)+ENLN(J)+TM)*EN(J,NPT)
      SS = H-F
      TERM1 = H
      IF (KMAT .EQ. IQ2) TERM1 = F
      DO 55 I = 1, L
C
C     CALCULATE THE ELEMENTS  R(I,K)
C
      IF (A(I,J) .EQ. 0.) GO TO 55
      TERM= A(I,J)*EN(J,NPT)
      DO 15  K=I, L
      G(I,K)= G(I,K) + A(K,J)*TERM
   15 CONTINUE
C
      G(I,IQ1)=G(I,IQ1)+TERM
      G(I,IQ2)=G(I,IQ2)+A(I,J)*TERM1
```

```
      IF (CONVG .OR.TP) GO TO 55
      G(I,IQ3)= G(I,IQ3)+A(I,J)*F
      IF (SP) G(IQ2,I) = G(IQ2,I) + A(I,J)*SS
   55 CONTINUE
      IF (KMAT .EQ. IQ2) GO TO 64
      IF(CONVG.OR.HP) GO TO 59
      G(IQ2,IQ1) = G(IQ2,IQ1) + SS
      G(IQ2,IQ2)=G(IQ2,IQ2)+H0(J)*SS
      G(IQ2,IQ3) = G(IQ2,IQ3)+(S(J) - ENLN(J)-TM)*F
      GO TO 62
   59 G(IQ2,IQ2)=G(IQ2,IQ2)+H0(J)*H
      IF (CONVG) GO TO 64
      G(IQ2,IQ3)=G(IQ2,IQ3)+H0(J)*F
   62 G(IQ1,IQ3)=G(IQ1,IQ3)+F
   64 G(IQ1,IQ2)=G(IQ1,IQ2)+TERM1
      GO TO 65
C
C     CONDENSED SPECIES
C
   70 KK = KK + 1
      DO 75  I = 1,L
      G(I,KK) = A(I,J)
      G(I,KMAT) = G(I,KMAT) - A(I,J)*EN(J,NPT)
   75 CONTINUE
      G(KK,IQ2) = H0(J)
      G(KK,KMAT) = H0(J) - S(J)
      HSUM(NPT) = HSUM(NPT)+ H
      IF(.NOT.SP) GO TO 65
      SSS = SSS + S(J)*EN(J,NPT)
      G(IQ2,KK) = S(J)
   65 CONTINUE
      SSS = SSS + G(IQ2,IQ1)
      HSUM(NPT) = HSUM(NPT) + G(IQ1,IQ2)
      G(IQ1,IQ1) = SUMN - ENN
C
C     REFLECT SYMMETRIC PORTIONS OF THE MATRIX
C
      ISYM = IQ1
      IF(HP.OR.CONVG)ISYM=IQ2
      DO 102 I=1,ISYM
      DO 102 J=I,ISYM
      G(J,I)=G(I,J)
  102 CONTINUE
C
C     COMPLETE THE RIGHT HAND SIDE
C
      IF(CONVG)  GO TO 175
      DO 145 I=1,L
      X(I)=B0(I)-G(I,IQ1)
      G(I,KMAT) = G(I,KMAT)+X(I)
  145 CONTINUE
      G(IQ1,KMAT) = G(IQ1,KMAT)+ENN-SUMN
C
C     COMPLETE ENERGY ROW AND TEMPERATURE COLUMN
C
      IF (KMAT .EQ. IQ2) GO TO 185
      IF (SP)ENERGY = S0+ENN-SUMN - SSS
      IF(HP)ENERGY=HSUB0/TT - HSUM(NPT)
      G(IQ2,IQ3)=G(IQ2,IQ3)+ ENERGY
  175 G(IQ2,IQ2)= G(IQ2,IQ2)+CPSUM
```

```
185 RETURN                                                    MAT*1200
    END                                                       MAT*1210
```

```
      SUBROUTINE MGAUSD
C
C     SOLVE ANY LINEAR SET OF UP TO 20 EQUATIONS
C
      DOUBLE PRECISION G,X,COEFX(20),SUM,Z
C
      COMMON/DOUBLE/G(20,21),X(20)
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,NLM
     1  ,N3,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
     2  ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK
C
      EQUIVALENCE (IUSE,IMAT)
C
      DATA BIGNO/1.E+38/
C
C     BEGIN ELIMINATION OF NNTH VARIABLE
C
      IUSE1=IUSE+1
    6 DO 45 NN=1,IUSE
      IF (NN-IUSE) 8,83,8
   83 IF(G(NN,NN))31,25,31
C
C     SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW
C
    8 DO 18 I=NN,IUSE
      COEFX(I) = BIGNO
      IF(G(I,NN).EQ.0.)  GO TO 18
      COEFX(I) = 0.
      DO 10 J=NN,IUSE1
      SUM = G(I,J)
      IF(SUM.LT.0.)  SUM=-SUM
      IF(J.NE.NN)  GO TO 9
      Z = SUM
      GO TO 10
    9 IF(SUM.GT.COEFX(I))  COEFX(I)=SUM
   10 CONTINUE
      COEFX(I) = COEFX(I)/Z
   18 CONTINUE
      TEMP = BIGNO
      I=0
   20 DO 22 J=NN,IUSE
      IF (COEFX(J)-TEMP) 87,22,22
   87 TEMP=COEFX(J)
      I=J
   22 CONTINUE
      IF(I) 28,23,28
C
C     INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NTH
C     VARIABLE FROM THE REMAINING EQUATIONS
C
C      INTERCHANGE EQUATIONS I AND NN
C
   28 IF(NN-I) 29,31,29
   29 DO 30 J=NN,IUSE1
      Z=G(I,J)
      G(I,J)=G(NN,J)
      G(NN,J)=Z
   30 CONTINUE
C
C     DIVIDE NTH ROW BY NTH DIAGONAL ELEMENT AND ELIMINATE THE NTH
```

```
C     VARIABLE FROM THE REMAINING EQUATIONS
C
   31 K = NN + 1
      DO 36 J = K, IUSE1
      IF(G(NN,NN).EQ.0.)  GO TO 23
            G(NN,J) = G(NN,J) / G(NN,NN)
   36 CONTINUE
      IF(K-IUSE1) 88,45,88
   88 DO 44 I = K,IUSE
   40 DO 44 J = K, IUSE1
            G(I,J) = G(I,J) - G(I,NN)*G(NN,J)
   44 CONTINUE
   45 CONTINUE
C
C     BACKSOLVE FOR THE VARIABLES
C
      K = IUSE
   47 J = K + 1
      X(K) = 0.0D0
      SUM = 0.0
      IF(IUSE - J) 51,48,48
   48 DO 50 I = J,IUSE
            SUM = SUM + G(K,I)* X(I)
   50 CONTINUE
   51 X(K) = G(K,IUSE1) - SUM
      K = K - 1
      IF (K) 47,151,47
   23 IUSE = IUSE-1
  151 RETURN
      END
```

```
      SUBROUTINE VARFMT(V,NPT)
C
      DIMENSION V(13)
C
      COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)
     1  ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2
     2  ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0
C
      DO 45 I=1,NPT
      K= 2*I+3
      FMT(K) = F4
      IF (V(I).GE.10.) FMT(K) = F3
      IF (V(I).GE.100.) FMT(K) = F2
      IF (V(I).GE.10000.)FMT(K) = F1
      IF (V(I).GE.1000000.) FMT(K) = F0
   45 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE OUT1
C
      DOUBLE PRECISION G,X
      REAL MIX(50)
      LOGICAL EQL,FROZ ,TP,HP,SP,HPSP,TPSP,MOLES
C
      DIMENSION NV(13),Z(10,3),HEAD(15),YX(5),YN(5)
      DIMENSION SIEGEL(30),CONCKI(10,30)
C
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)
     2  ,TOTN(13)
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)
     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
     4 ,RHOP,RMW(15),TLN
      COMMON /DOUBLE/ G(20,21), X(20)
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,NLM
     1  ,NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK
      COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13)
     1 ,CPRF(13),AEAT(13),CSTR,EGL,FROZ,SS0
      COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)
     1   ,FC(4),FG(4),F8,FMT13,F1,F2,F3,F4,F5,FL(4),FMT19,FA1,FA2
     2   ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0
      COMMON/SNEW/RON,INDFA
      COMMON/EQNEW/R1(30,40),R6(30,40),EK1(30,40),EK2(30,40),ROH(30,40),
     1CH2(30,40),ATT(13,40),F(40),PHI(40),BCON1(30,40),BCON2(30,40),BCON
     26(30,40)
C
      EQUIVALENCE (V,NV),(Z,H0),(I8,F8)
C
C     HEAD=(1H ,2A4,5  (A2,F8.5,3X),5  X,F7.5,F13.3,4X,A1,F10.2,F9.4)
C
      DATA HEAD/4H(1H ,4H,2A4,2H,5,4H(A2,,4HF8.5 ,4H,3X),2H,5 ,2HX,
     1     ,4HF7.5 ,4H,F13 ,4H.3,4 ,4HX,A1 ,4H,F10 ,4H.2,F ,4H9.4)/
      DATA FUEL/4HFUEL/,OXID/4HOXID/,ANT/3HANT/,OX/1HO/,IZ/2H00/
     1       ,YN/2H,1, 2H,2, 2H,3, 2H,4, 2H,5 /,F75/4HF7.5/
     2       ,YX/3H,57,3H,44,3H,31,3H,18,2H,5 /,F73/4HF7.3/
      DATA(SIEGEL(I),I=1,30)/4HC(S),4H    ,4H    ,4HCO  ,4H    ,4H    ,4
     1HCO2 ,4H    ,4H    ,4HH   ,4H    ,4H    ,4HN   ,4H    ,4H    ,4HNO
     2 ,4H    ,4H    ,4HN2O ,4H    ,4H    ,4HO   ,4H    ,4H    ,4HO2  ,4
     3H    ,4H    ,4HOH  ,4H    ,4H    /

      IF(KASE.NE.0) WRITE (6,3) KASE
    3 FORMAT (9H CASE NO. ,I5)
      IF(.NOT.MOLES) WRITE(6,5)
    5 FORMAT (77X,46HWT FRACTION  ENTHALPY  STATE    TEMP     DENSITY/
     1 10X,16HCHEMICAL FORMULA,51X,21H(SEE NOTE)     CAL/MOL,10X,5HDEG K,
     2 4X,4HG/CC )
      IF(MOLES) WRITE(6,6)
    6 FORMAT (79X,5HMOLES,7X,  33HENTHALPY  STATE    TEMP     DENSITY/
     1 10X,16HCHEMICAL FORMULA,66X,7HCAL/MOL,10X,13HDEG K     G/CC )
      DO 15 N=1,NREAC
      IF(FOX(N).NE.OX)GO TO 10
      HD1 = OXID
      HD2 = ANT
```

```
      GO TO 11
   10 HD1 = FUEL
      HD2 = FB
   11 DO 13 J=1,5
      IF(NAME(N,J).EQ.IZ.OR.NAME(N,J).EQ.IB)  GO TO 14
   13 CONTINUE
      J=6
   14 J=J-1
      HEAD(3)=YN(J)
      HEAD(7)=YX(J)
      HEAD(9) = F75
      IF(PECWT(N).GE.10.)  HEAD(9)=F73
      WRITE(6,HEAD)HD1,HD2,(NAME(N,JJ),ANUM(N,JJ),JJ=1,J),PECWT(N),ENTH(
     1N), FAZ(N),RTEMP(N),DENS(N)
   15 CONTINUE
      FPC = 100./(1.+OF)
      WRITE(6,20)  OF   ,FPC,EQRAT,RHOP
   20 FORMAT (1H0,15X, 4HO/F=, F9.4,3X,13HPERCENT FUEL=,F8.4,4X,
     1  19HEQUIVALENCE RATIO= ,F7.4,4X,9HDENSITY=,F8.4//)
C
      AGV = 9.80665
      RETURN
C
      ENTRY OUT2
C
C   PRESSURE
C
      FMT(4)= FMT(6)
      CALL VARFMT (PPP ,NPT)
      WRITE (6,FMT)(FP(I),I=1,4),(PPP(J),J=1,NPT)
C
C   TEMPERATURE
C
      DO 65 I=1,NPT
      NV(I)= TTT(I)+.5
   65 CONTINUE
      FMT(4)= FMTI3
      FMT(5)= FMTI9
      WRITE (6,FMT)(FT(I),I=1,4),(NV(J),J=1,NPT)
C
C   ENTHALPY
C
      DO 75 I=1,NPT
      V(I) = HSUM(I) * R
   75 CONTINUE
      FMT(5)= F8
      FMT(7)= F1
      WRITE (6,FMT)(FH(I),I=1,4),(V(J),J=1,NPT)
C
C   ENTROPY
C
      FMT(7)=F4
      DO 78 I = 1,NPT
      V(I) = SSUM(I) * R
   78 CONTINUE
      WRITE (6,FMT)(FS(I),I=1,4),(V(J),J=1,NPT)
      WRITE (6,80)
   80 FORMAT ( 1H )
C
C   MOLECULAR WEIGHT
```

```
C
      FMT(7)= F3
      WRITE (6,FMT)(FM(I),I=1,4),(WM(J),J=1,NPT)
C
C    (DLV/DLP)T
C
      FMT(7)=F5
      IF(EQL) WRITE(6,FMT)(FV(I),I=1,4),(DLVPT(J),J=1,NPT)
C
C    (DLV/DLT)P
C
      FMT(7)= F4
      IF(EQL) WRITE(6,FMT)(FD(I),I=1,4),(DLVTP(J),J=1,NPT)
C
C    HEAT CAPACITY
C
      DO 85  I=1,NPT
      V(I) = CPR(I) * R
   85 CONTINUE
      WRITE(6,FMT)(FC(I),I=1,4),(V(J),J=1,NPT)
C
C    GAMMA(S)
C
      WRITE(6,FMT)(FG(I),I=1,4),(GAMMAS(J),J=1,NPT)
C
C    SONIC VELOCITY
C
      FMT(7)= F1
      DO 95 I = 1,NPT
      SONVEL(I) = SQRT(RR*GAMMAS(I)*TTT(I)/WM(I))
   95 CONTINUE
      WRITE(6,FMT)(FL(I),I=1,4),(SONVEL(J),J=1,NPT)
      RETURN
C
      ENTRY OUT3
      IF(.NOT.EQL)  GO TO 331
      DO 309 I = 1,NPT
      DATA (I) = 0.
      DO 308 K = 1,NS
      DATA(I) = DATA(I) + EN(K,I)
  308  CONTINUE
  309 CONTINUE
C
C    MOLE FRACTIONS - EQUILIBRIUM
C
      WRITE (6,80)
      FMT(7)= F5
      WRITE(6,310)
  310 FORMAT(15H0MOLE FRACTIONS //)
      DO 330 K=1,NS
      DO 315 I=1,NPT
      V(I) = EN(K,I) / DATA (I)
  315 CONTINUE
      DO 316 I=1,NPT
      IF (V(I).GE.(5.E-6)) GO TO 320
  316 CONTINUE
      GO TO 330
  320 WRITE (6,FMT) SUB(K,1),SUB(K,2),SUB(K,3),FB,(V(I),I=1,NPT)
  330 CONTINUE
  331 WRITE(6,335)
```

```
335 FORMAT(118H0ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOOUT*1800
   1LE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS//)OUT*1810
    LINE= 0                                                            OUT*1820
    NN = 1                                                             OUT*1830
    IF(EQL)  NN=NPT                                                    OUT*1840
    DO 350 K=1,NS                                                      OUT*1850
    DO 340  I=1,NN                                                     OUT*1860
    IF ((EN(K,I)/DATA(I)).GE.(5.E-6)) GO TO 343                        OUT*1870
340 CONTINUE                                                           OUT*1880
    LINE= LINE+1                                                       OUT*1890
    Z(LINE ,1)= SUB(K,1)                                               OUT*1900
    Z(LINE,2)= SUB(K,2)                                                OUT*1910
    Z(LINE,3)= SUB(K,3)                                                OUT*1920
343 IF ((LINE.NE.10) .AND. K.NE.NS) GO TO 350                          OUT*1930
    IF (LINE.EQ.0) GO TO 1000                                          OUT*1940
    WRITE(6,345) (Z(LN,1),Z(LN,2),Z(LN,3),LN=1,LINE)                   OUT*1950
345 FORMAT (10(1X,3A4))                                                OUT*1960
    LINE= 0                                                            OUT*1970
350 CONTINUE                                                           OUT*1980
    IF(.NOT.MOLES) WRITE(6,360)                                        OUT*1990
360 FORMAT(78H0NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIOUT*2000
   2DANT IN TOTAL OXIDANTS    )                                        OUT*2010
1000 CONTINUE                                                          OUT*2020
    DO 3000 I =1,10                                                    OUT*2030
    II = 3*I - 2                                                       OUT*2040
    DO 2000 K =1,NS                                                    OUT*2050
    IF(SIEGEL(II).NE.SUB(K,1)) GO TO 2000                              OUT*2060
    IF(SIEGEL(II+1).NE.SUB(K,2)) GO TO 2000                            OUT*2070
    IF(SIEGEL(II+2).NE.SUB(K,3)) GO TO 2000                            OUT*2080
    DO 1500 J =1,NPT                                                   OUT*2090
1500 CONCKI(I,J) = EN(K,J)/DATA(J)                                     OUT*2100
    GO TO 3000                                                         OUT*2110
2000 CONTINUE                                                          OUT*2120
3000 CONTINUE                                                          OUT*2130
C****                                                                  OUT*2140
C**** NOTE...FOR MORE THAN NPT=6,THESE PRINT STATEMENTS MUST BE MODIFIEDOUT*2150
C****                                                                  OUT*2160
    DO 5000 K=1,10                                                     OUT*2170
    II = 3*K - 2                                                       OUT*2180
    WRITE(6,4000) SIEGEL(II),SIEGEL(II+1),SIEGEL(II+2),(CONCKI(K,J),J=OUT*2190
   11,NPT)                                                             OUT*2200
4000 FORMAT(1X,3A4,2X,6(E15.8,1X))                                     OUT*2210
5000 CONTINUE                                                          OUT*2220
    WRITE(6,6000) (WM(J),J =1,NPT)                                     OUT*2230
6000 FORMAT(11H MOLEC. WT.,4X,6(E15.8,1X))                             OUT*2240
    WRITE(6,7000) (TTT(J),J=1,NPT)                                     OUT*2250
7000 FORMAT(9H TEMP.(K),6X,6(E15.8,1X)                                 OUT*2260
    WRITE(6,8000) (PPP(J),J=1,NPT)                                     OUT*2270
8000 FORMAT(12H PRESS.(ATM),3X,6(E15.8,1X))                            OUT*2280
    WRITE(6,9000) RON                                                  OUT*2290
9000 FORMAT(14H FUEL AIR RAT.,1X,E15.8)                                OUT*2300
    DO 9600 N =1,NREAC                                                 OUT*2310
    WRITE(6,9500) (ANUM(N,JJ),JJ=1,5),ENTH(N),RTEMP(N)                 OUT*2320
9500 FORMAT(1X,7E15.8)                                                 OUT*2330
9600 CONTINUE                                                          OUT*2340
    CALL RATES(CONCKI,WM,TTT,PPP,ANUM,ENTH,RTEMP,NPT,NREAC)            OUT*2350
9999 RETURN                                                            OUT*2360
    END                                                                OUT*2370
```

```
      SUBROUTINE RATES(CONCKI,WM,TTT,PPP,ANUM,ENTH,RTEMP,NPT,NREAC)
      REAL MIX(50)
      DIMENSION CONCKI(10,30),TTT(13),PPP(13),WM(13),ANUM(15,5),ENTH(15)
     1,RTEMP(15)
      DIMENSION R2(30,40),R3(30,40),R4(30,40),R5(30,40),RATEK(6,30,40),C
     1ONMCM(10,30,40),A(6),EN(6),E(6)
      COMMON/SNEW/RON,INDFA
      COMMON/DICK/MIX
      COMMON/EQNEW/R1(30,40),R6(30,40),EK1(30,40),EK2(30,40),ROH(30,40),
     1CH2(30,40),ATT(13,40),F(40),PHI(40),BCON1(30,40),BCON2(30,40),BCON
     26(30,40)
      DATA(A(I),I=1,6)/3.1E+13,6.4E+09,4.1E+13,2.9513E+13,3.8146E+13,4.5
     1775E+13/,(EN(I),I=1,6)/0.,1.,0.,0.,0.,0./,(E(I),I=1,6)/0.334E+00,6
     2.250E+00,0.0E+00,10.77E+00,24.1E+00,24.1E+00/,ICODE/2/
C****
C**** TEST FOR WRITE CONTROL
C****
      IST = INDFA
      IPRINT = 0
      IF(MIX(IST+1).EQ.0.0) IPRINT = 1
C****
C**** SET PRESSURE LOOP
C****
      DO 8000 J = 1,NPT
C****
C**** CALCULATE CONCENTRATIONS
C****
      BCON1(J,IST) = CONCKI(1,J)
      BCON2(J,IST) = CONCKI(2,J)
      BCON6(J,IST) = CONCKI(6,J)
      DO 1000 I = 1,10
      CONMCM(I,J,IST) = (CONCKI(I,J)*PPP(J))/(82.057*TTT(J))
 1000 CONTINUE
C****
C**** COMPUTE RATE CONSTANTS
C****
      DO 2000 I =1,6
      RATEK(I,J,IST) = A(I)*(TTT(J)**EN(I))*EXP(-E(I)/(1.987E-03*TTT(J))
     1)
 2000 CONTINUE
C****
C**** CALCULATE FORWARD REACTION CONSTANTS
C****
      R1(J,IST) = (RATEK(1,J,IST)*CONMCM(5,J,IST)*CONMCM(6,J,IST))
      R2(J,IST) = (RATEK(2,J,IST)*CONMCM(5,J,IST)*CONMCM(9,J,IST))
      R3(J,IST) = (RATEK(3,J,IST)*CONMCM(5,J,IST)*CONMCM(10,J,IST))
      R4(J,IST) = (RATEK(4,J,IST)*CONMCM(4,J,IST)*CONMCM(7,J,IST))
      R5(J,IST) = (RATEK(5,J,IST)*CONMCM(8,J,IST)*CONMCM(7,J,IST))
      R6(J,IST) = (RATEK(6,J,IST)*CONMCM(8,J,IST)*CONMCM(7,J,IST))
C****
C**** CALCULATE K1,K2,RHO,KS, AND PHI
C****
      IF(R2(J,IST).EQ.0.0.AND.R3(J,IST).EQ.0.0) EK1(J,IST) = 1.0E+35
      IF(R2(J,IST).EQ.0.0.AND.R3(J,IST).EQ.0.0) GO TO 2500
      EK1(J,IST) = (R1(J,IST)/(R2(J,IST)+R3(J,IST)))
 2500 IF(R4(J,IST).EQ.0.0.AND.R5(J,IST).EQ.0.0) EK2(J,IST) = 1.0E+35
      IF(R4(J,IST).EQ.0.0.AND.R5(J,IST).EQ.0.0) GO TO 2750
      EK2(J,IST) = (R6(J,IST)/(R4(J,IST)+R5(J,IST)))
 2750 ROH(J,IST) = (PPP(J)*WM(J))/(82.057*TTT(J))
C****
```

```
C****  NOTE...FUEL CARD IS PHYSICALLY BEFORE OXIDANT CARD IN INPUT,OXYGEN
C****  IS SECOND SPECIE SPECIFIED IN OXIDANT AIR,FUEL IS SPECIFIED C-A,
C****  H-8
C****
       EKS = ((12.*ANUM(1,1)+1.*ANUM(1,2))*ANUM(2,2))/(28.99*(ANUM(1,1)+(
      1ANUM(1,2)/4.)))
       PHI(IST) =  RON/EKS
       F(IST) = PHI(IST)*EKS/(1.+(PHI(IST)*EKS))
C****
C****  CALCULATE CONCENTRATION OF CH2
C****
       RATWTS = ANUM(1,1)/ANUM(1,2)
       CH2(J,IST) = (((RATWTS/(1.+12.*RATWTS))*(WM(J)*RON/(RON+1.)))-CONC
      1KI(2,J)-CONCKI(3,J)-CONCKI(1,J))
C****
C****  STOPE VALUES OF T
C****
       ATT(J,IST) = TTT(J)
  8000 CONTINUE
C****
C****  PRINT AND PUNCH OUTPUT
C****
       IF(IPRINT.EQ.0) GO TO 9999
       DO 9500 J = 1,NPT
       DO 9000 I =1,IST
       IF(I.NE.1) GO TO 8500
       WRITE(6,8100) ANUM(1,1),ANUM(1,2),RTEMP(2),PPP(J),ICODE,EKS
       WRITE(7,8100) ANUM(1,1),ANUM(1,2),RTEMP(2),PPP(J),ICODE,EKS
  8100 FORMAT(1X,7HFUEL= C,E15.8,1HH,E15.8,18H INLET AIR T.(K)= ,E15.8/1X
      1,13HPRESS.(ATM)= ,E15.8,7HICODE= ,I2,13HPHI STOICH.= ,E15.8)
  8500 WRITE(6,8200) F(I),PHI(I),ROH(J,I),ATT(J,I),BCON6(J,I),BCON2(J,I),
      1BCON1(J,I),CH2(J,I),R1(J,I),R6(J,I),EK1(J,I),EK2(J,I)
  8200 FORMAT(1X,6E12.5/1X,6E12.5)
       WRITE(7,8250) F(I),PHI(I),ROH(J,I),ATT(J,I),BCON6(J,I),BCON2(J,I),
      1BCON1(J,I),CH2(J,I),R1(J,I),R6(J,I),EK1(J,I),EK2(J,I)
  8250 FORMAT(6E12.5/6E12.5)
  9000 CONTINUE
  9500 CONTINUE
  9999 RETURN
       END
```

```
      SUBROUTINE HCALC
C
C  CALCULATE ENTHALPY FOR PROPELLANT USING COEFFICIENTS
C
      LOGICAL MOLES
      DIMENSION NUM(15,5)
C
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)
     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
     4 ,RHOP,RMW(15),TLN
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,NLM
     1  ,NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK
C
      EQUIVALENCE (ANUM,NUM),(L,NLM),(J,JS1)
C
      DATA AG/1HG/,IZERO/2H00/,OX/1HO/,BLK/1H /
C
C  IS TT IN RANGE
C
      IF(TT.LT.(TLOW-100.).OR.TT.GT.(THIGH+1000.))GO TO 75
      HPP(1)=0.
      HPP(2)=0.
      AC(1)=0.
      AC(2)=0.
      DO 900 N=1,NREAC
      K=2
      IF(FOX(N).EQ.OX)K=1
      PCWT=PECWT(N)
      IF(MOLES)PCWT=PCWT*RMW(N)
      IF(NAME(N,5).EQ.IZERO)GO TO 5
      AC(1) = 0.
      AC(2) = 0.
      GO TO 500
    5 J   = NUM(N,5)
      IF (J.NE.0)  GO TO 90
      DO 10 J=1,L
      DATA(J)=0.
   10 CONTINUE
      DO 40 I=1,4
      IF(ANUM(N,I).EQ.0.)GO TO 50
      DO 20 J=1,L
      IF(LLMT(J).EQ.NAME(N,I)) GO TO 30
   20 CONTINUE
   30 DATA(J)=ANUM(N,I)
   40 CONTINUE
   50 IS=0
      DO 70 J=1,NS
      IF(IUSE(J).EQ.0)GO TO 55
      IS = IS+1
      IF(FAZ(N).EQ.AG)GO TO 70
      IF(TT.GT.TEMP(IS,2).AND.TEMP(IS,2).NE.THIGH)  GO TO 70
      IF(TT.LT.TEMP(IS,1).AND.TEMP(IS,1).NE.TLOW)  GO TO 70
      GO TO 56
   55 IF(FAZ(N).NE.AG.AND.FAZ(N).NE.BLK)  GO TO 70
   56 DO 60 I=1,L
```

```
      IF(A(I,J).NE.DATA(I))  GO TO 70
   60 CONTINUE
      NUM(N,5) = J
      GO TO 90
   70 CONTINUE
      GO TO 80
   90 NSS = NS
      NS = J
      DELN(J)= EN(J,NPT)
      EN(J,NPT) = 1.
      CALL CPHS
      EN(J,NPT) = DELN(J)
      NS = NSS
      IF (HO(J).GT.-.01 .AND. HO(J).LT..01) HO(J) = 0.
      RTEMP(N) = TT
      ENTH(N) = HO(J)*R*TT
      AC(K)=AC(K)+CPSUM*PCWT/RMW(N)
  500 HPP(K)=HPP(K)+ENTH(N)*PCWT/RMW(N)
  900 CONTINUE
      IF(.NOT.MOLES)  GO TO 951
      DO 950 K=1,2
      IF(WP(K).EQ.0.)GO TO 950
      HPP(K)=HPP(K)/WP(K)
      AC(K)=AC(K)/WP(K)
  950 CONTINUE
  951 HSUB0 = (OF*HPP(1) + HPP(2))/(OF+1.)
      GO TO 1000
   75 WRITE(6,76)
   76 FORMAT(50H0REACTANT TEMPERATURE OUT OF RANGE OF THERMO DATA )
   80 WRITE(6,85) N
   85 FORMAT(1H0,I2,34H TH REACTANT IS NOT IN THERMO DATA )
 1000 RETURN
      END
```

```
      SUBROUTINE MOLIER
C
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)
     2,TOTN(13)
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)
     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
     4 ,RHOP,RMW(15),TLN
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,NLM
     1   ,NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK
      DO 91 IT = 1,26
      IF (T(IT).EQ. 0.) GO TO 95
      NT = IT
   91 CONTINUE
C
C     SET ASSIGNED P
C
   95 DO 902 IP = 1,NP
      PP = P(IP)
C
C     SET ASSIGNED T
C
      DO 902 IT=1,NT
      TT = T(IT)
      CALL EQLBRM
      IF(TT.NE.0.)  GO TO 800
      IF(NPT.EQ.0)  GO TO 1000
  800 K = 0
      IF(IP.EQ.NP.AND.IT.EQ.NT.OR.TT.EQ.0.)  GO TO 860
      K = NPT
      IF(NPT.NE.13)  GO TO 870
  860 WRITE (6,5)
    5 FORMAT(1H1,41X,48HTHERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED
     1     ,/53X,28H TEMPERATURES AND PRESSURES    ///  )
      CALL OUT1
      WRITE (6,863)
  863 FORMAT (25H0THERMODYNAMIC PROPERTIES//)
      CALL OUT2
      CALL OUT3
  865 IF(K.EQ.0) GO TO 1000
      WRITE(6,868)
  868 FORMAT(1H1)
      NPT = 0
  870 NPT = NPT + 1
C
C   SAVE COMPOSITIONS FOR ESTIMATES OF NEXT POINT
C
      DO 880 I = 1,NS
      EN(I,NPT) = EN(I,K)
  880 CONTINUE
  902 CONTINUE
 1000 RETURN
      END
```

```
      SUBROUTINE CMBSTN
C
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)
     2,TOTN(13)
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)
     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
     4 ,RHOP,RMW(15),TLN
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,NLM
     1   ,NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK
C
C     SET ASSIGNED P
C
      TT = 3800.
      DO 902 IP = 1,NP
      PP = P(IP)
      CALL EQLBRM
      T(NPT) = TT
      IF(TT.NE.0.)  GO TO 800
      IF(NPT.EQ.0)  GO TO 1000
  800 K=0
      IF(IP.EQ.NP.OR.TT.EQ.0.)  GO TO 860
      K = NPT
      IF(NPT.NE.13)  GO TO 870
  860 WRITE (6,6)
    6 FORMAT (1H1,42X,48HTHEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES
     1   ///)
      CALL OUT1
      WRITE (6,863)
  863 FORMAT (25H0THERMODYNAMIC PROPERTIES//)
      CALL OUT2
      CALL OUT3
  865 IF(K.EQ.0) GO TO 1000
      NPT = 0
  870 NPT = NPT + 1
C
C
C    SAVE COMPOSITIONS FOR ESTIMATES OF NEXT POINT
      DO 880 I = 1,NS
      EN(I,NPT) = EN(I,K)
  880 CONTINUE
  902 CONTINUE
 1000 RETURN
      END
```

```
      SUBROUTINE DETON
C
C     CHAPMAN-JOUGUET DETONATIONS
C
      LOGICAL HP,SP,TP,IDEBUG,NEWR,IONS,MOLES,FROZ,EQL,PSIA,RKT
      LOGICAL CPCVEQ, CPCVFR, CALCH
C
      DIMENSION GM(13),CP(13),H1(13),PUB(13),TUB(13),GM1(13),RRHO(13)
C
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)
     2  ,TOTN(13)
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)
     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
     4 ,RHOP,RMW(15),TLN
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,NLM
     1  ,NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
     2 ,IONS,NC,ASERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK
      COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13)
     1 ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SS0
      COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)
     1  ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMT19,FA1,FA2
     2  ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0
C
      EQUIVALENCE(CP,DATA),(GM,SPIM),(H1,VAC1),(PUB,SUBAR),(TUB,SUPAR)
      EQUIVALENCE(GM1,AEAT),(PCP(14),RRHO)
C
      DATA FT1/4HT1,D/, FP1/4HP1,A/, FH1/4HH1,C/, FM1/4HM1,M/
     1 ,  FCP1/4HCP1,/, FG1/4HA1  /, FPP/4HP/P1/, FTT/4HT/T1/
     2 ,   FUD/4HDET /, FMM/4HM/M1/, FRA/4HRHO//, FRB/4HRHO1/
     3 ,   FMA/4HMACH/, FMB/4H NO./, IZERO/2H00/
C
      D(C)= A11*A22-A21*A12
      XX(Y)= (B1*A22-B2*A12)/D(C)
      YY(Z)= (B2*A11-B1*A21)/D(C)
C
      NT = 1
      HSUB0 = HSUB0*R
      CALCH   .FALSE.
      TT = 0.
      IF(T(1).EQ.0.)  T(1)=RTEMP(1)
      DO 2 N = 1,NREAC
      IF(NAME(N,5).EQ.IZERO) CALCH = .TRUE.
    2 CONTINUE
      DO 3  IT = 1,26
      IF (T(IT).EQ.0.) GO TO 7
      NT = IT
    3 CONTINUE
    7 IF (AM(1).NE.0.0 .AND. AM(2).NE.0.0) GO TO4
      AM1 = AM(2)
      IF (AM(2).EQ.0.0)AM1 = AM(1)
      GO TO 9
    4 AM1 = (OF+1.)*AM(2)*AM(1)/(AM(1) +OF*AM(2))
    9 WRITE (6,11)
   11 FORMAT(33H1DETONATION VELOCITY CALCULATIONS)
      DO 903 IT=1,NT
```

```
      T1= T(IT)
      TT = T1
      IF (.NOT.CALCH)  GO TO 15
      CALL HCALC
      CALL OUT1
   15 CP1 = (OF*AC(1) + AC(2))/(OF+1.)
      DO 902 IP=1,NP
      P1= P(IP)
      H1(NPT) = HSUB0
      TUB(NPT)=T1
      PUB(NPT)=P1
      CP(NPT) = CP1*R
      ITR= 0
      TT= 3800.
      PP1= 15.
      PP= PP1*P1
      HSUB0 = H1(NPT)/R + .75*T1*PP1/AM1
      TP = .FALSE.
      HP= .TRUE.
      CALL EQLBRM
      HSUB0 = H1(NPT)
      HP= .FALSE.
      IF(TT.EQ.0.) GO TO 1000
      GAM= GAMMAS(NPT)
      TT1= TT/T1
      II= 0
      TEM=TT1-.75*PP1/(CPR(NPT)*AM1)
      AMM=WM(NPT)/AM1
      WRITE(6,190)TT
  190 FORMAT(8HOT EST.=,F8.2/11X,4HP/P1,17X,4HT/T1)
      WRITE(6,203) II,PP1,TT1
C
  200 DO 202 II=1,4
      ALFA=AMM/TT1
      PP1= (1.+GAM)*(1.+(1.-4.*GAM*ALFA/(1.+GAM)**2)**.5)/(2.*GAM*ALFA)
      RK=PP1*ALFA
      TT1= TEM+.5*PP1*GAM*(RK*RK-1.)/(AM1*CPR(NPT)*RK)
      WRITE(6,203) II,PP1,TT1
  203 FORMAT (I5,2E20.8)
  202 CONTINUE
      TP= .TRUE.
      TT= T1*TT1
      RR1 = PP1*AMM/TT1
C
  205 ITR= ITR+1
      PP= P1*PP1
      CALL EQLBRM
      IF (NPT.EQ.0) GO TO 1000
      IF (TT.EQ.0.) GO TO 860
      GAM= GAMMAS(NPT)
C     IF(CPCVFR)GAM= CPRF(NPT)/(CPRF(NPT)-1./WM(NPT))
C     IF(CPCVEQ)GAM= -GAMMAS(NPT)*DLVPT(NPT)
      AMM= WM(NPT)/AM1
      RR1= PP1*AMM/TT1
      A11= 1./PP1 + GAM*RR1*DLVPT(NPT)
      A12= GAM*RR1*DLVTP(NPT)
      A21= .5*GAM*(RR1**2-1.-DLVPT(NPT)*(1.+RR1**2))+DLVTP(NPT)-1.
      A22=-.5*GAM*DLVTP(NPT)*(RR1**2+1.)-WM(NPT)*CPR(NPT)
      B1= 1./PP1-1.+GAM*(RR1-1.)
      B2= WM(NPT)*(HSUM(NPT)-H1(NPT)/R)/TT-.5*GAM*(RR1*RR1-1.)
```

```
      X1 = XX(Y)
      X2 = YY(Z)
      ALAM= 1.
      TEM = X1
      IF(TEM.LT.0.)  TEM = -TEM
      IF(X2.GT.TEM)  TEM=X2
      IF (-X2.GT.TEM) TEM = -X2
      IF(TEM.GT.0.4) ALAM=.4/TEM
      PP1= PP1*EXP(X1*ALAM)
      TT1= TT1*EXP(X2*ALAM)
      TT = T1*TT1
      US = (RR*GAM*TT/WM(NPT))**.5
      UD= RR1*US
      WRITE(6,10) ITR
   10 FORMAT (21H0   ITERATION NUMBER=I2      )
      WRITE(6,30) PP1,TT1,RR1,X1,X2,US
   30 FORMAT(6X,4HP/P1,10X,1H= E20.8/6X,4HT/T1,10X,1H= E20.8/6X,8HRHO/RH
     101,6X,1H= E20.8/6X,11HDEL LN P/P1,3X,1H=E20.8/6X,11HDEL LN T/T1,3X
     2,1H=E20.8/6X,2HUS,12X,1H=E20.8)
C
C     CONVERGENCE TEST
C
      IF(ITR.LE.10 .AND. TEM.GT.0.5E-04)  GO TO 205
      RRHO(NPT)=RR1
      IF (CP(NPT).EQ.0.) GO TO 40
      GM1(NPT) = CP(NPT) /(CP(NPT)-R/AM1)
      VMOC(NPT) = UD/(RR*GM1(NPT)*T1/AM1)**.5
      GO TO 41
   40 GM1(NPT) = 0.
      VMOC(NPT) = 0.
      GO TO 150
C
C  DERIVATIVES
C
   41 WRITE(6,55)
   55 FORMAT (                17H0   DERIVATIVE OF,13X,4HLN P,16X,4HLN T
     1,16X,2HUD,              /9X,2HBY )
      B1= 1./PP1-GAM*RR1
      B2= GAM*RR1**2
      X1 = XX(Y)
      X2 = YY(Z)
      AA= .5*(1.-DLVPT(NPT))
      BB= -.5*DLVTP(NPT)
      DUD= UD*(AA*X1+BB*X2-1.)
      X1= X1-1.0
      WRITE(6,81)X1,X2,DUD
   81 FORMAT(6X,13HLNP1 AT T1,HI,6X,1H=,3E17.8 )
      B1= GAM*RR1
      B2= -B1*RR1-WM(NPT)*CP(NPT)/(R*TT1)
      X1 = XX(Y)
      X2 = YY(Z)
      DUD= UD*(AA*X1+BB*X2+1.)
      X2= X2-1.
      WRITE(6,84)X1,X2,DUD
   84 FORMAT(6X,16HLNT1 AT P1,HI,M1,3X,1H=3E17.8)
      B1= 0.
      B2= -WM(NPT)/(R*TT)
      X1 = XX(Y)*1000.
      X2 = YY(Z)*1000.
      DUD= UD*(AA*X1+BB*X2)
```

```
      WRITE(6,85)X1,X2,DUD
   85 FORMAT (6X,20HH)    AT T1,P1,H1    =3E17.8)
C
  150 K = 0
      IF(IP.EQ.2.AND.IT.EQ.NT.OR.TT.EQ.0.)  GO TO 650
      K = NPT
      IF(NPT.NE.13)  GO TO 870
C
C  OUTPUT
C
  860 WRITE (6,5)
    5 FORMAT(1H1,42X,46HDETONATION PROPERTIES OF AN IDEAL REACTING GAS )
      CALL OUT1
      WRITE(6,46)
   46 FORMAT(13H UNBURNED GAS//)
      FMT(4)=FMT13
      FMT(5)=F8
      FMT(7)=F4
      WRITE(6,FMT)FP1,FP(2),FB,FB,(PUB(J),J=1,NPT)
      FMT(7)=F2
      WRITE(6,FMT)FT1,FT(2),FB,FB,(TUB(J),J=1,NPT)
      WRITE(6,FMT)FH1,FH(2),FB,FB,(H1(J), J=1,NPT)
      DO 56 I=1,NPT
      V(I)=AM1
      SONVEL(I)=    (RR*GM1(I)*TUB(I)/AM1)**.5
   56 CONTINUE
      FMT(7)=F3
      WRITE(6,FMT) FM1,FM(2),FM(3),FB,(V(J),J=1,NPT)
      FMT(7)=F4
      WRITE(6,FMT)FCP1,FC(2),FC(3),FC(4),(CP(J),J=1,NPT)
      WRITE(6,FMT)FG(1),FG1,FB,FB,(GM1(J),J=1,NPT)
      FMT(7)=F1
      WRITE(6,FMT)(FL(I),I=1,4),(SONVEL(J),J=1,NPT)
      WRITE(6,58)
   58 FORMAT(11H0BURNED GAS//)
      FMT(4)=FMT(6)
      CALL OUT2
      WRITE(6,68)
   68 FORMAT(22H0DETONATION PARAMETERS //)
      FMT(7)=F3
      DO 70 I=1,NPT
      V(I)= PPP(I)/PUB(I)
      PCP(I)=TTT(I)/TUB(I)
      SONVEL(I)=SONVEL(I)*RRHO(I)
   70 CONTINUE
      WRITE(6,FMT)FPP,FB,FB,FB,(V(J),J=1,NPT)
      WRITE(6,FMT)FTT,FB,FB,FB,(PCP(J),J=1,NPT)
      DO 73 I=1,NPT
      V(I)=WM(I)/AM1
   73 CONTINUE
      FMT(7)=F4
      WRITE(6,FMT)FMM,FB,FB,FB,(V(J),J=1,NPT)
      WRITE(6,FMT)FRA,FRB,FB,FB,(RRHO(J),J=1,NPT)
      WRITE(6,FMT)FMA,FMB,FB,FB,(VMOC(J),J=1,NPT)
      FMT(7)=F1
      WRITE(6,FMT) FUD,FL(2),FL(3),FL(4),(SONVEL(J),J=1,NPT)
      EOL=.TRUE.
      CALL OUT3
  865 IF(K.EQ.0) GO TO 1000
      WRITE(6,868)
```

```
  868 FORMAT(1H1)
      NPT = 0
  870 NPT = NPT + 1
C
C   SAVE COMPOSITIONS FOR ESTIMATES OF NEXT POINT
C
      DO 880 I = 1,NS
      EN(I,NPT) = EN(I,K)
  880 CONTINUE
      WRITE (6,868)
  902 CONTINUE
  903 CONTINUE
 1000 TP = .FALSE.
      RETURN
      END
```

```
      SUBROUTINE SHCK                                                   SHC*0000
      RETURN                                                            SHC*0010
      END                                                               SHC*0020
```

```
      SUBROUTINE ROCKET
C
C     ROCKET PERFORMANCE
C     EITHER HPSP OR TPSP IS TRUE
C
      LOGICAL HP,SP,TP,IDEBUG,NEWR ,IONS,MOLES,FROZ,EQL,LOGV,HPSP,TPSP
C
      DIMENSION AA(2),BB(2),CC(2)
C
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)
     2,TOTN(13)
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)
     1 ,DELN(150),X(15,150),SUB(150,3),IUSE(150),TEMP(50,2)
      COMMON/MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),BOP(15,2)
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AC(2),AM(2)
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
     4 ,RHOP,RMW(15),TLN
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,NLM
     1   ,NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK
      COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13)
     1 ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SSO
C
      NAMELIST/RKTINP/EQL,FROZ,SUBAR,SUPAR,PCP
C
      ITH = 0
  210 DO 300 I=1,26
      PCP(I)= 0.
      SUBAR(I) = 0.
  300 CONTINUE
      TT = 3800.
      HPSP = .TRUE.
      HP = .TRUE.
      TPSP = .FALSE.
      EQL = .TRUE.
      FROZ = .TRUE.
      READ (5,RKTINP)
      IF (T(1) .EQ.0.) GO TO 303
      TPSP = .TRUE.
      TT = T(1)
      TP = .TRUE.
      HPSP = .FALSE.
  303 IF(PCP(1).NE.0.)  GO TO 308
      DO 305  I=1,NP
      K = NP-I+2
      P(K) = P(K-1)
  305 CONTINUE
      GO TO 311
  308 NP= 2
      DO 310 I=1,24
      IF (I.GT.2) GO TO 309
      IF ((PCP(I).EQ.0.).OR.PCP(I).EQ.1.) GO TO 310
  309 IF (PCP(I).EQ.0.) GO TO 311
      NP = NP + 1
      P(NP) = P(1)/PCP(I)
  310 CONTINUE
  311 NSUB=0
      NSUP = 0
```

```
      DO 320  I=1,13
      IF(SUBAR(I).NE.0.)NSUB=NSUB+1
      IF(SUPAR(I).NE.0.)NSUP=NSUP+1
  320 CONTINUE
      WRITE (6,RKTINP)
      SS0 = 0.
      ITROT=.3
C
C     SET ASSIGNED P
C
      DO 902 IP = 1,NP
      PP = P(IP)
      CALL EQLBRM
      IF(TT.NE.0.)  GO TO 333
      IF(NPT.EQ.0)  GO TO 1000
      GO TO 900
  333 PCP(NPT) = P(1)/PP
      IF(IP.GT.1)  GO TO 195
C
C     COMBUSTION CHAMBER
C
      TP = .FALSE.
      HP = .FALSE.
      SP = .TRUE.
      S0 = SSUM(1)
      PCP(2)=((GAMMAS(1)+1.)/2.)**(GAMMAS(1)/(GAMMAS(1)-1.))
      P(2) = P(1)/PCP(2)
      TT = 2.*TT/(GAMMAS(1)+1.)
      GO TO 900
  195 IF(IP.GT.2) GO TO 900
C
C     THROAT
C
  190 IF(ITH.NE.2)  GO TO 191
      ITH = 0
      GAMMAS(2) = 0.
      GO TO 900
  191 DH = HSUM(1)-HSUM(2)
      DHSTAR = DH-GAMMAS(2)*TT*ENN/2.
      IF (IDEBUG) WRITE(6,923)DHSTAR,HSUM(1),HSUM(2),PCP(2)
  923 FORMAT(4E25.8)
      DH = DHSTAR/DH
      IF(DH.LT.0.)  DH=-DH
      IF(DH.LE.0.4E-4.OR.ITROT.EQ.0)  GO TO 900
      IF(JSOL.NE.0) ITH =1
      IF (JSOL.EQ.0.AND.ITH.EQ.1) ITH=2
      IF(ITH.EQ.0) GO TO 192
C
C     SPECIAL THROAT INTERPOLATION IF ITH = 2
C
      DLNI = .5*TT*ENN/(HSUM(1)-HSUM(2))
      AA(ITH)=.5*DLNI*(2.*DLNI+(GAMMAS(2)-1.)/GAMMAS(2))
      XX = ALOG(PCP(2))
      BB(ITH) = 1./GAMMAS(2)-DLNI-2.*XX*AA(ITH)
      CC(ITH) = ENN*TT/(PP*(HSUM(1)-HSUM(2))**.5)
      CC(ITH) = ALOG(CC(ITH))-XX*(BB(ITH)+AA(ITH)*XX)
      IF(ITH.EQ.1)  GO TO 192
      BB(1)=BB(1)-BB(2)
      AA(1)=AA(1)-AA(2)
      PCP(2)=(-BB(1)+(BB(1)*BB(1)-4.*AA(1)*(CC(1)-CC(2)))**.5)/(2.*AA(1)
```

```
     1)                                                          RCK*1200
      PCP(2)=EXP(PCP(2))                                         RCK*1210
      GO TO 193                                                  RCK*1220
  102 PCP(2)= PCP(2)/(1.+2.*DHSTAR/(ENN*TT *(GAMMAS(2)+1.)))     RCK*1230
  193 P(2) = P(1) / PCP(2)                                       RCK*1240
      PP = P(2)                                                  RCK*1250
      ITROT = ITROT+1                                            RCK*1260
      CALL EQLBRM                                                RCK*1270
      IF(TT.EQ.0.) GO TO 1000                                    RCK*1280
      GO TO 190                                                  RCK*1290
C                                                                RCK*1300
  900 K = 0                                                      RCK*1310
      IF (.NOT.EQL .AND. FROZ) GO TO 990                         RCK*1320
      IF(IP.EQ.NP.OR.TT.EQ.0.)  GO TO 860                        RCK*1330
      K = NPT                                                    RCK*1340
      IF(NPT.NE.13)  GO TO 870                                   RCK*1350
  860 CALL RKTOUT                                                RCK*1360
      IF ((NSUB + NSUP).NE.0) CALL RATIO                         RCK*1370
      IF(K.EQ.0) GO TO 990                                       RCK*1380
      WRITE(6,865)                                               RCK*1390
  865 FORMAT(1H1)                                                RCK*1400
      NPT = 2                                                    RCK*1410
  870 NPT = NPT + 1                                              RCK*1420
C                                                                RCK*1430
C   SAVE COMPOSITIONS FOR ESTIMATES OF NEXT POINT                RCK*1440
C                                                                RCK*1450
      DO 880 I = 1,NS                                            RCK*1460
      EN(I,NPT) = EN(I,K)                                        RCK*1470
  880 CONTINUE                                                   RCK*1480
  902 CONTINUE                                                   RCK*1490
  990 IF (FROZ) CALL FROZEN                                      RCK*1500
 1000 RETURN                                                     RCK*1510
      END                                                        RCK*1520
```

```
      SUBROUTINE RKTOUT
C
C  ROCKET PERFORMANCE PARAMETERS
C
      LOGICAL EQL,FROZ ,TP,HP,SP,HPSP,TPSP,SHOCK
C
      DIMENSION NV(13),Z(10,4)
C
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)
     2  ,TOTN(13)
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)
     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
     2 ,HPF(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
     4 ,RHOP,RMW(15),TLN
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,NLM
     1   ,NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK
      COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13)
     1 ,CPRF(13),AFAT(13),CSTR,EQL,FROZ,SS0
      COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)
     1  ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2
     2  ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0
C
      EQUIVALENCE (V,NV),(Z,H0)
C
      DATA EXIT/4HEXIT/
C
      IF(EQL) WRITE (6,37)
   37 FORMAT(1H1/24X,84HTHEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBR
     1IUM COMPOSITION DURING EXPANSION         //)
      IF (.NOT.EQL) WRITE (6,38)
   38 FORMAT(1H1,26X,78HTHEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN C
     1OMPOSITION DURING EXPANSION         //)
      IF (TPSP) WRITE (6,737)
  737 FORMAT (52X,28HAT AN ASSIGNED TEMPERATURE
      V(1) = PPP(1)*14.696006
      WRITE (6,40) V(1)
   40 FORMAT(5H PC = ,F8.1,5H PSIA)
      CALL OUT1
      NEX = NPT - 2
      DO 862 I = 1,NEX
  862 V(I) = EXIT
      WRITE(6,48) (V(I),I=1,NEX)
   48 FORMAT(1H0,16X,16HCHAMBER   THROAT  ,11(5X,A4))
C
C     PRESSURE RATIO
C
      FMT(4) = FMT(6)
      CALL VARFMT (PCP,NPT)
      WRITE (6,FMT) FR1,FB,FB,FB,(PCP(J),J=1,NPT)
      CALL OUT2
C
      AGV = 9.80665
      DO 202 K=2,NPT
      SPIM(K) = (2.*RR*(HSUM(1)-HSUM(K)))**.5/AGV
C
```

```
C  AW (A/W) IN UNITS OF SEC/ATM
C
      AW = RR*TTT(K)/(PPP(K)*                WM(K)*SPIM(K)*AGV**2)
      IF(K.NE.2)GO TO 200
      AWT=AW
      CSTR=32.174*P(1)*AWT
  200 AEAT(K)=AW/AWT
      VACI(K)=SPIM(K)+PPP(K)*AW
      IF (SONVEL(K).NE.0.) VMOC(K)=SPIM(K)*AGV/SONVEL(K)
      NV(K)= CSTR + .5
  202 CONTINUE
C
C   MACH NUMBER
C
      VMOC(1)=0.
      IF(GAMMAS(2).EQ.0.) VMOC(2)=0.
      FMT(7) = F3
      WRITE(6,FMT)(FN(I),I=1,4),(VMOC(J),J=1,NPT)
      WRITE (6,208)
  208 FORMAT (1H )
C
C   C*
C
      FMT(4) = FMT9X
      FMT(5) = FMT13
      FMT(6) = FMTI9
      FMT(7) = F8
      WRITE(6,FMT)(FR(I),I=1,4),(NV(J),J=2,NPT)
C
C   CF - THRUST COEFICIENT
C
      FMT(6) = FMT(8)
      FMT(7) = F3
      DO 212  I=2,NPT
  212 V(I)=32.174*SPIM(I)/CSTR
      WRITE(6,FMT)FC1,F8,F8,F8,(V(J),J=2,NPT)
C
C   AREA RATIO
C
      CALL VARFMT (AEAT,NPT)
      FMT(5) = F8
      WRITE(6,FMT)FA1,FA2,F8,F8,(AEAT(J),J=2,NPT)
C
C   VACUUM IMPULSE
C
      FMT(5) = FMT13
      FMT(7) = F1
      WRITE(6,FMT)(FA(I),I=1,4),(VACI(J),J=2,NPT)
C
C   SPECIFIC IMPULSE
C
      WRITE(6,FMT)(FI(I),I=1,4),(SPIM(J),J=2,NPT)
      WRITE (6,208)
      FMT(4) = F8
      FMT(5) = FMT13
      FMT(7) = F5
      IF(EQL)  GO TO 312
      WRITE(6,310)
  310 FORMAT(15H0MOLE FRACTIONS //)
C
```

```
C   MOLE FRACTIONS - FROZEN
C
      DO 309 I=1,NPT
      DATA(I) = 0.
      DO 308 K=1,NS
      DATA(I) = DATA(I)+EN(K,I)
  308 CONTINUE
  309 CONTINUE
      LINE = 0
      DO 430 K =1,NS
      V(LINE+1) = EN(K,1)/DATA(1)
      IF (V(LINE+1).LT.(5.E-6))  GO TO 424
      LINE = LINE+1
      Z(LINE,1) = SUB(K,1)
      Z(LINE,2) = SUB(K,2)
      Z(LINE,3) = SUB(K,3)
      Z(LINE,4) = V(LINE)
  424 IF (LINE.NE.4.AND.K.NE.NS)  GO TO 430
      IF (LINE.EQ.0)  GO TO 312
      WRITE (6,426) (Z(LN,1),Z(LN,2),Z(LN,3),Z(LN,4),LN=1,LINE)
  426 FORMAT (1H ,4(3A4,F9.5,7X))
      LINE = 0
  430 CONTINUE
  312 CALL OUT3
 1000 RETURN
      END
```

```
      SUBROUTINE RATIO
C
C     (USED FOR AREA RATIO INTERPOLATION ONLY)
C
      DOUBLE PRECISION G,X
      LOGICAL EQL, FROZ,TPSP
C
      DIMENSION PER(2,2),AI(13),APCP(13),AT(13),AMWT(13),RP(2),NV(13)
     1 , RPP(2)
C
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)
     2,TOTN(13)
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)
     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)
      COMMON/MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
     4 ,RHOP,RMW(15),TLN
      COMMON /DOUBLE/ G(20,21), X(20)
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,NLM
     1  ,NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK
      COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13)
     1 ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SS0
      COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)
     1  ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMT19,FA1,FA2
     2  ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0
C
      EQUIVALENCE (V,NV)
C
      NBLO = NPT-2
      DO 22 J=3,NPT
      IF(PCP(J).GT.PCP(2))GO TO 30
   22 CONTINUE
      GO TO 31
   30 NBLO=J-3
   31 DO 1200  ISONIC=1,2
      LL = 1
      IF(ISONIC.EQ.2)  GO TO 34
      IF(NSUB.EQ.0)  GO TO 1200
      NAR = NSUB
      GO TO 36
   34 IF(NSUP.EQ.0)  GO TO 1200
      NAR = NSUP
   36 DO 1100 I=1,NAR
      IF(ISONIC.EQ.2)  GO TO 40
      IF(NBLO.LE.1) GO TO 1100
      K=2+NBLO
      DO 38 J=4,K
      V(LL) = SUBAR(I)
      IF(V(LL).GE.AEAT(J)) GO TO 56
   38 CONTINUE
      GO TO 56
   40 IF(NPT-NBLO.LE.3)  GO TO 1100
      V(LL) = SUPAR(I)
      K=4+NBLO
      DO 42 J=K,NPT
      IF(V(LL).LE.AEAT(J))  GO TO 56
```

```
   42 CONTINUE
      IF(V(LL).GE.AEAT(J)*3.)  GO TO 85
   56 KJ = J-1
      K = KJ
      DO 64 JJ=1,2
      IF(CPR(K).NE.0.)  GO TO 63
      WRITE(6,62)K
   62 FORMAT(17HOCANNOT USE POINT,I2,3X,4HCP=0 )
      GO TO 1100
   63 PER(JJ,1)=-1./(CPR(K)*WM(K))
      IF (EQL) PER(JJ,1) =  PER(JJ,1)*DLVTP(K)
      PER(JJ,2)=   TTT(K)/(2.*WM(K)*(HSUM(1)-HSUM(K)))
      RP(JJ) = 1./(1./GAMMAS(K)-PER(JJ,2))
      IF(EQL)RPP(JJ) = 1.+DLVPT(K)+(1.-DLVTP(K))*PER(JJ,1)
      K = KJ + 1
   64 CONTINUE
      AMWT(LL) = WM(1)
      CALL SET(PCP(KJ),RP(1),AEAT(KJ),V(LL),    APCP(LL))
      CALL SET(TTT(KJ),PER(1,1),PCP(KJ),APCP(LL),AT(LL))
      IF(EQL)CALL SET (WM(KJ),RPP(1),PCP(KJ),APCP(LL),AMWT(LL))
      K = KJ
      DO 74 JJ=1,2
      G(JJ,7)=SPIM(K)**2
      G(JJ+2,7)=2.*G(JJ,7)*PER(JJ,2)
      G(JJ+4,7)=(1.-GAMMAS(K))/GAMMAS(K)*G(JJ+2,7)
      G(JJ,1)=1.
      G(JJ+2,1)= 0
      G(JJ+4,1)=0
      G(JJ,2)=ALOG(PCP(K))
      G(JJ+2,2)=1.
      G(JJ+4,2)=0
      DO 70 M=3,6
      G(JJ,M)=G(JJ,2)**(M-1)
      G(JJ+2,M)=G(JJ,2)**(M-2)*FLOAT(M-1)
      G(JJ+4,M)=G(JJ+2,M)/G(JJ,2)*FLOAT(M-2)
   70 CONTINUE
      K = KJ + 1
   74 CONTINUE
      IMAT = 6
      CALL MGAUSD
      AI(LL)= X (1)
      DO 84 JJ=2,6
      AI(LL)=AI(LL)+ X (JJ)*ALOG(APCP(LL))**(JJ-1)
   84 CONTINUE
      IF(AI(LL).LE.0.)GO TO 85
      AI(LL) = AI(LL)**.5
      GO TO 86
   85 LL = LL - 1
   86 IF(LL.GE.13.OR.I.GE.NAR) GO TO 90
      LL = LL+1
      GO TO 1100
C
C     OUTPUT
C
   90 IF(EQL) WRITE (6,87)
   87 FORMAT(1H1/24X,84HTHEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBR
     1IUM COMPOSITION DURING EXPANSION            //)
      IF (.NOT.EQL) WRITE (6,88)
   88 FORMAT(1H1,26X,78HTHEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN C
     1OMPOSITION DURING EXPANSION          //)
```

```
      IF (TPSP) WRITE (6,99)
   99 FORMAT (52X,28HAT AN ASSIGNED TEMPERATURE
      WRITE (6,91)
   91 FORMAT (52X,24HFOR ASSIGNED AREA RATIOS     //)
      PC= P(1)*14.696006
      WRITE(6,191)PC
  191 FORMAT(5H PC = ,F8.1,5H PSIA)
      CALL OUT1
      IF(ISONIC.EQ.1) WRITE(6,33)
   33 FORMAT(18H0SUBSONIC FLOW      //)
      IF (ISONIC.EQ.2) WRITE (6,35)
   35 FORMAT(18H0SUPERSONIC FLOW    //)
C
C     AREA RATIO
C
      FMT(6)= FMT(8)
      FMT(4)= FMT(6)
      CALL VARFMT (V,NPT)
      WRITE(6,FMT) FA1,FA2,FB,FB,(V(M),M=1,LL)
C
C     VACUUM SPECIFIC IMPULSE AND SPECIFIC IMPULSE
C
      DO 93 M=1,LL
      V(M)=AI(M)+CSTR*V(M)/(32.174* APCP(M))
   93 CONTINUE
      FMT(4)= FMT13
      FMT(5)= FB
      FMT(7)= F1
      WRITE(6,FMT) (FA(N),N=1,4), (V(M),M=1,LL)
      WRITE(6,FMT) (FI(N),N=1,4), (AI(M),M=1,LL)
C
C     C*
C
      FMT(5)= FMT19
      DO 94 M=1,LL
      NV(M)=CSTR +.5
   94 CONTINUE
      WRITE(6,FMT) (FR(N),N=1,4), (NV(M),M=1,LL)
C
C     CF - THRUST COEFFICIENT
C
      DO 95 M=1,LL
      V(M)=AI(M)*32.174/CSTR
   95 CONTINUE
      FMT(5)= FB
      FMT(7)= F3
      WRITE(6,FMT) FC1,FB,FB,FB,(V(M),M=1,LL)
      WRITE(6,96)
   96 FORMAT(1H )
C
C     PRESSURE RATIO
C
      FMT(4)= FMT(6)
      CALL VARFMT (APCP,NPT)
C

      CALL VARFMT (APCP,NPT)
C
C     PRESSURE
C
```

```
      WRITE(6,FMT) FR1,FR,FB,FB,(APCP(M),M=1,LL)
      DO 98  M=1,LL
      V(M) = P(1)/APCP(M)
   98 CONTINUE
      CALL VARFMT (V,NPT)
      WRITE(6,FMT) (FP(N),N=1,4), (V(M),M=1,LL)
C
C     TEMPERATURE
C
      DO 101 M=1,LL
      NV(M)=AT(M)+.5
  101 CONTINUE
      FMT(4)= FMTI3
      FMT(5)= FMTI9
      WRITE(6,FMT) (FT(N),N=1,4), (NV(M),M=1,LL)
C
C     ENTHALPY
C
      FMT(5)= FB
      FMT(7)= F1
      DO 104 M=1,LL
      V(M)= HSUM(1)*R-1000.*(AI(M)/294.98)**2
  104 CONTINUE
      WRITE(6,FMT) (FH(N),N=1,4), (V(M),M=1,LL)
C
C     ENTROPY
C
      FMT(7)=F4
      V(1) = SSUM(2)*R
      DO 106 M=1,LL
      V(M) = V(1)
  106 CONTINUE
      WRITE(6,FMT) (FS(N),N=1,4), (V(M),M=1,LL)
C
C     MOLECULAR WEIGHT
C
      FMT(7)=F3
      WRITE(6,FMT) (FM(N),N=1,4), (AMWT(M),M=1,LL)
 1100 CONTINUE
 1200 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE SET(ONE,TWO,THREE,ARG,HAL)
C
C     (USED FOR AREA RATIO INTERPOLATION ONLY)
C     SETS UP ALL 4 BY 5 MATRICES
C
      DOUBLE PRECISION A,ANS,G,X
C
      DIMENSION ANS(6),ONE(2),TWO(2),THREE(2),A(20,21)
C
      COMMON /DOUBLE/ G(20,21), X(20)
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,NLM
     1  ,NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK
C
      EQUIVALENCE (G,A),(X,ANS)
C
      DO 8 J=1,2
      A(J,5)=ALOG(ONE(J))
      A(J+2,5)=TWO(J)
      A(J,2)=ALOG(THREE(J))
    8 CONTINUE
      DO 1 I=1,2
      A(I,1)=1.0
      A(I+2,1)=0.0
      A(I+2,2)=1.0
      DO 1 J=2,3
      A(I,J+1)=A(I,2)**J
      A(I+2,J+1)=A(I,2)**(J-1)*FLOAT(J)
    1 CONTINUE
      IMAT = 4
      CALL MGAUSD
      HAL=ANS(1)
      SUM=ALOG(ARG)
      DO 10 J=1,3
      HAL=HAL+SUM**J*(ANS(J+1))
   10 CONTINUE
      HAL=EXP(HAL)
      RETURN
      END
```

```
      SUBROUTINE FROZEN
C
C     (FROZEN COMPOSITION EXPANSION ONLY)
C
      LOGICAL EQL,FROZ,CONVG
C
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)
     2,TOTN(13)
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)
     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBC,AC(2),AM(2)
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
     4 ,RHOP,RMW(15),TLN
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,NLM
     1   ,NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK
      COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13)
     1 ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SS0
      COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)
     1   ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMT19,FA1,FA2
     2   ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0
      ITROT = 3
      EQL =.FALSE.
      NPT = 2
       TT = TTT(1)
      TLN=ALOG(TT)
      GAMMAS(1) = CPRF(1)/(CPRF(1)-1./WM(1))
      CPR(1) = CPRF(1)
      PCP(2) = ((GAMMAS(1)+1.)/2.)**(GAMMAS(1)/(GAMMAS(1)-1.))
      DATA(1) = 2./(GAMMAS(1) + 1.)
      TLN = TLN + ALOG(DATA(1))
      DO 902  IP=2,NP
      IF(NPT.EQ.2)  GO TO 45
      PCP(NPT) = P(1)/P(IP)
   45 CONVG = .FALSE.
      PCPLN= ALOG(PCP(NPT))
      S0 = SS0 -PCPLN/WM(1)
      SUMH = 0.
   51 TT=EXP(TLN)
      SUMS=0.
      JS1 = 1
      NNN = NPT
      NPT = 1
      CALL CPHS
      NPT = NNN
      DO 60 J=1,NS
      IF(EN(J,1).EQ.0.)  GO TO 60
      SUMS = SUMS + S(J)*EN(J,1)
      IF(CONVG) SUMH=SUMH+H0(J)*EN(J,1)
   60 CONTINUE
      IF (CONVG) GO TO 81
      DLNT=(SUMS-S0)/CPSUM
      TLN=TLN-DLNT
      IF(DLNT.LT.0.) DLNT=-DLNT
      IF(DLNT.LT.0.5E-4)  CONVG=.TRUE.
      GO TO 51
   81 TTT(NPT)= TT
```

```
      SSUM(NPT)= SSUM(1)                                              FRZ*0600
      HSUM(NPT)= TT*SUMH                                              FRZ*0610
      GAMMAS(NPT)= CPSUM/(CPSUM-1./WM(1))                             FRZ*0620
      IF(IP.GT.2)  GO TO 90                                           FRZ*0630
C                                                                     FRZ*0640
C     THROAT CALCULATIONS                                             FRZ*0650
C                                                                     FRZ*0660
      DH = HSUM(1)-HSUM(2)                                            FRZ*0670
      DHSTAR = DH-(GAMMAS(2)*TT/(2.*WM(1)))                           FRZ*0680
      DH = DHSTAR/DH                                                  FRZ*0690
      IF(DH.LT.0.)  DH=-DH                                            FRZ*0700
      IF(DH.LE.0.4E-4.OR.ITROT.EQ.0) GO TO 90                         FRZ*0710
      PCP(2) = PCP(2)/(1.+2.*DHSTAR*WM(1)/(TT*(GAMMAS(2)+1.)))        FRZ*0720
      P(2) = P(1)/PCP(2)                                              FRZ*0730
      ITROT = ITROT-1                                                 FRZ*0740
      GO TO 45                                                        FRZ*0750
   90 WM(NPT)= WM(1)                                                  FRZ*0760
      PPP(NPT) = P(IP)                                                FRZ*0770
      CPR(NPT)= CPSUM                                                 FRZ*0780
      K = 0                                                           FRZ*0790
      IF (TT.LT.(TLOW-150.))GO TO 903                                 FRZ*0800
      IF(NC.EQ.0) GO TO 700                                           FRZ*0810
      INC =0                                                          FRZ*0820
      DO 901 I=1,NS                                                   FRZ*0830
      IF(IUSE(I).EQ.0.OR.IUSE(I).EQ.-10000) GO TO 901                 FRZ*0840
      INC = INC+1                                                     FRZ*0850
      IF(EN(I,1).EQ.0.) GO TO 901                                     FRZ*0860
      IF (TT.LT.(TEMP(INC,1)-50.).OR.TT.GT.(TEMP(INC,2)+50.))GO TO 903 FRZ*0870
  901 CONTINUE                                                        FRZ*0880
  700 IF ( IP.EQ.NP) GO TO 863                                        FRZ*0890
      K = NPT                                                         FRZ*0900
      IF (NPT.NE.13) GO TO 870                                        FRZ*0910
      GO TO 863                                                       FRZ*0920
  903 NPT = NPT - 1                                                   FRZ*0930
  863 CALL RKTOUT                                                     FRZ*0940
      IF (NSUB*NSUP.NE.0) CALL RATIO                                  FRZ*0950
  865 IF (K.EQ.0) GO TO 1000                                          FRZ*0960
      NPT = 2                                                         FRZ*0970
  870 NPT = NPT + 1                                                   FRZ*0980
  902 CONTINUE                                                        FRZ*0990
 1000 RETURN                                                          FRZ*1000
      END                                                             FRZ*1010
```

```
      BLOCK DATA
C
      DIMENSION ATEM(3,50)
C
      COMMON/MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),BOP(15,2)
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AC(2),AM(2)
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
     4 ,RHOP,RMW(15),TLN
      COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)
     1  ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2
     2  ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0
C
      EQUIVALENCE (ATOM(1,52),ATEM)
C
C  ATOMIC SYMBOLS, WEIGHTS, AND VALENCES
C
      DATA ATOM/
     A    2HH ,  1.00797, 1.,    2HHE,  4.0026, 0.,    2HLI,  6.939   , 1.,
     B    2HBE,  9.0122 , 2.,    2HB , 10.811 , 3.,    2HC , 12.01115, 4.,
     C    2HN , 14.0067 , 3.,    2HO , 15.9994,-2.,    2HF , 18.9984 ,-1.,
     D    2HNE, 20.183  , 0.,    2HNA, 22.9898, 1.,    2HMG, 24.312  , 2.,
     E    2HAL, 26.9815 , 3.,    2HSI, 28.086 , 4.,    2HP , 30.9738 , 5.,
     F    2HS , 32.064  , 4.,    2HCL, 35.453 ,-1.,    2HAR, 39.948  , 0.,
     G    2HK , 39.102  , 1.,    2HCA, 40.080 , 2.,    2HSC, 44.956  , 3.,
     H    2HTI, 47.900  , 4.,    2HV , 50.942 , 5.,    2HCR, 51.996  , 3.,
     I    2HMN, 54.9380 , 2.,    2HFE, 55.847 , 3.,    2HCO, 58.9332 , 2.,
     J    2HNI, 58.710  , 2.,    2HCU, 63.540 , 2.,    2HZN, 65.370  , 2.,
     K    2HGA, 69.720  , 3.,    2HGE, 72.590 , 4.,    2HAS, 74.9216 , 3.,
     L    2HSE, 78.960  , 4.,    2HBR, 79.909 ,-1.,    2HKR, 83.800  , 0.,
     M    2HRB, 85.47   , 1.,    2HSR, 87.620 , 2.,    2HY , 88.905  , 3.,
     N    2HZR, 91.220  , 4.,    2HNB, 92.906 , 5.,    2HMO, 95.94   , 6.,
     O    2HTC, 99.000  , 7.,    2HRU,101.070 , 3.,    2HRH,102.905  , 3.,
     P    2HPD,106.400  , 2.,    2HAG,107.870 , 1.,    2HCD,112.400  , 2.,
     Q    2HIN,114.820  , 3.,    2HSN,118.690 , 4.,    2HSB,121.750  , 3. /
      DATA ATEM/
     R    2HTE,127.600  , 4.,    2HI ,126.9044,-1.,    2HXE,131.300  , 0.,
     S    2HCS,132.905  , 1.,    2HBA,137.340 , 2.,    2HLA,138.910  , 3.,
     T    2HCE,140.120  , 3.,    2HPR,140.907 , 3.,    2HND,144.240  , 3.,
     U    2HPM,145.000  , 3.,    2HSM,150.350 , 3.,    2HEU,151.960  , 3.,
     V    2HGD,157.250  , 3.,    2HTB,158.924 , 3.,    2HDY,162.500  , 3.,
     W    2HHO,164.930  , 3.,    2HER,167.260 , 3.,    2HTM,168.934  , 3.,
     X    2HYB,173.040  , 3.,    2HLU,174.997 , 3.,    2HHF,178.490  , 4.,
     Y    2HTA,180.948  , 5.,    2HW ,183.850 , 6.,    2HRE,186.200  , 7.,
     Z    2HOS,190.200  , 4.,    2HIR,192.200 , 4.,    2HPT,195.090  , 4.,
     A    2HAU,196.967  , 3.,    2HHG,200.590 , 2.,    2HTL,204.370  , 1.,
     B    2HPB,207.190  , 2.,    2HBI,208.980 , 3.,    2HPO,210.000  , 2.,
     C    2HAT,210.000  , 0.,    2HRN,222.000 , 0.,    2HFR,223.000  , 1.,
     D    2HRA,226.000  , 2.,    2HAC,227.000 , 3.,    2HTH,232.038  , 4.,
     E    2HPA,231.000  , 5.,    2HU ,238.030 , 6.,    2HNP,237.000  , 5.,
     F    2HPU,242.000  , 4.,    2HAM,243.000 , 3.,    2HCM,247.000  , 3.,
     G    2HBK,249.000  , 3.,    2HCF,251.000 , 3.,    2HES,254.000  , 0.,
     H    2HFM,253.000  , 0.,    2HMV,256.000 , 0./
C
C     INFORMATION USED IN VARIABLE OUTPUT FORMAT
C
      DATA FMT/3H(1H,4H,3A4,4H,A2,,3HF9.,1H ,3HF9.,1H ,3HF9.,1H ,3HF9.,1
     1H ,3HF9.,1H ,3HF9.,1H ,3HF9.,1H ,3HF9.,1H ,3HF9.,1H ,3HF9.,1H ,3HF
     29.,1H ,3HF9.,1H ,3HF9.,1H ,1H)/, F3,F0,F1,F2,F3,F4,F5/1H  ,2H0,,2H
     31,,2H2,,2H3,,2H4,,2H5,/,FMT13/2H13/,FMT9X/3H9X,/,FMTI9/3HI9,/
```

```
      DATA                              FP/4HP, A,4HTM  ,2H  ,1H /           BLK*0600
     1,FT/4HT, D,4HEG K,4H    ,2H  /,FH/4HH, C,4HAL/G,2H  ,1H /              BLK*0610
     2,FS/4HS, C,4HAL/(,4HG)(K,2H) /,FM/4HM, M,4HOL, W,2HT ,1H /             BLK*0620
     3,FV/4H(DLV,4H/DLP,4H)T  ,2H  /,FD/4H(DLV,4H/DLT,2H)P,1H /              BLK*0630
     4,FC/4HCP, ,4HCAL/,4H(G)(,2HK)/,FG/4HGAMM,4HA (S,2H) ,1H /              BLK*0640
     5,FL/4HSON ,4HVEL,,4HM/SE,2HC /                                         BLK*0650
C                                                                            BLK*0660
C     INFORMATION USED IN PERFORMANCE OUTPUT                                 BLK*0670
C                                                                            BLK*0680
      DATA FR1/4HPC/P/, FC1/2HCF/,    FN/4HMACH,4H NUM,4HBER ,1H /           BLK*0690
     1,FR/4HCSTA,4HR, F,4HT/SE,2HC  /,FI/4HI, L,4HB-SE,4HC/LB,1H /           BLK*0700
     2,FA/4HIVAC,4H,LB-,4HSEC/,2HLB /,FA1/4HAE/A/,FA2/1HT/                   BLK*0710
      END                                                                    BLK*0720
```

APPENDIX VII - LISTING OF THERMO DATA

```
THERMO
   300.000  1000.000  5000.000             FIRST CARD
ALCS)               J12/65AL  10   00   00   0S   300.000   933.000             1
 0.              0.              0.              0.              0.               2
 0.              0.              0.22258601E 01 0.25561698E-02 0.25963942E-06    3
-0.44923993E-05 0.38349536E-11-0.77250039E 03-0.10016767E 02                     4
AL(L)               J12/65AL  10   00   00   0L   933.000  5000.000             1
 0.38185052E 01 0.              0.              0.              0.               2
-0.95116844E 02-0.17518952E 02 0.38185052E 01 0.              0.               3
 0.              0.             -0.95116844E 02-0.17518952E 02                   4
AL                  J12/65AL  100  000  000  0G   300.000  5000.000             1
 0.25450650E 01-0.75157512E-04 0.48674178E-07-0.14045399E-10 0.15219285E-14    2
 0.38498357E 05 0.53100256E 01 0.27964983E 01-0.12468435E-02 0.20733316E-05    3
-0.15457769E-08 0.43185442E-12 0.39456100E 05 0.41365426E 01                     4
AL+                 J 6/65AL  1E   -100  000  0G   300.000  5000.000             1
 0.25138516E 01-0.29077490E-04 0.20604308E-07-0.59989578E-11 0.62050860E-15    2
 0.10559636E 06 0.37023323E 01 0.25006758E 01-0.44314947E-05 0.10158061E-07    3
-0.97918340E-11 0.33894328E-14 0.10860109E 06 0.37744969E 01                     4
ALBO2               J 6/66AL  1B   10   200  0G   300.000  5000.000             1
 0.71722995E 01 0.29780741E-02-0.12431107E-05 0.23188779E-09-0.16041208E-13    2
-0.67683532E 05-0.99949242E 01 0.23087234E 01 0.18590539E-01-0.20633348E-04    3
 0.10251324E-07-0.16941283E-11-0.66482167E 05 0.14463834E 02                     4
ALCL                J 9/64AL  1CL  100  000  0G   300.000  5000.000             1
 0.43754335E 01 0.18702767E-03-0.49969033E-07 0.55147171E-11-0.53213024E-15    2
-0.69880112E 04 0.23323888E 01 0.33327027E 01 0.44047734E-02-0.65385801E-05    3
 0.44387437E-08-0.11170643E-11-0.67755002E 04 0.73643189E 01                     4
ALCL+               J 6/68AL  1CL  1E   -10  0G   300.000  5000.000             1
 0.43738449E 01 0.19205255E-03-0.54247204E-07 0.85478382E-11-0.37491125E-15    2
 0.10231686E 06 0.31197190E 01 0.33759844E 01 0.42774116E-02-0.64051041E-05    3
 0.43882415E-08-0.11166597E-11 0.10251734E 06 0.79219510E 01                     4
ALCLF               J 9/64AL  1CL  1F   100  0G   300.000  5000.000             1
 0.64593361E 01 0.59530273E-03-0.25682111E-06 0.43695729E-10-0.34023629E-14    2
-0.62463694E 05-0.33724191E 01 0.35819421E 01 0.11405579E-01-0.15489628E-04    3
 0.93913221E-08-0.20431534E-11-0.61639641E 05 0.10712370E 02                     4
ALCLF2              J 9/64AL  1CL  1F   200  0G   300.000  5000.000             1
 0.89238843E 01 0.11946919E-02-0.51514910E-06 0.98204262E-10-0.68997466E-14    2
-0.12250084E 06-0.15879099E 02 0.42215332E 01 0.18167323E-01-0.23359617E-04    3
 0.13307895E-07-0.26426994E-11-0.12144555E 06 0.73068482E 01                     4
ALCL2               J 9/64AL  1CL  200  000  0G   300.000  5000.000             1
 0.66933063E 01 0.33723173E-03-0.14321882E-06 0.26838381E-10-0.18532160E-14    2
-0.39336262E 05-0.38121908E 01 0.43363468E 01 0.99563726E-02-0.15049433E-04    3
 0.10272735E-07-0.26037172E-11-0.39361237E 05 0.75382417E 01                     4
ALCL2+              J 6/68AL  1CL  2E   -10  0G   300.000  5000.000             1
 0.71787698E 01 0.34798442E-03-0.14533263E-06 0.26764431E-10-0.18162627E-14    2
 0.53103955E 05-0.95391313E 01 0.47027704E 01 0.10475953E-01-0.15939365E-04    3
 0.11000908E-07-0.28333967E-11 0.53608594E 05 0.23835549E 01                     4
ALCL2-              J 6/68AL  1CL  2E   10   0G   300.000  5000.000             1
 0.66765684E 01 0.35805640E-03-0.15322113E-06 0.28934079E-10-0.20128276E-14    2
-0.42352615E 05-0.44184290E 01 0.42601657E 01 0.10221323E-01-0.15461789E-04    3
 0.10586258E-07-0.26976715E-11-0.41365195E 05 0.72197011E 01                     4
ALCL2F              J 9/64AL  1CL  2F   100  0G   300.000  5000.000             1
 0.91351571E 01 0.90569395E-03-0.39032127E-06 0.74305714E-10-0.52114210E-14    2
-0.97369793E 05-0.15622927E 02 0.45609210E 01 0.17353741E-01-0.24017677E-04    3
 0.14983444E-07-0.34108047E-11-0.96939961E 05 0.54911550E 01                     4
ALCL3               J 3/64AL  1CL  300  000  0G   300.000  5000.000             1
 0.93997905E 01 0.67170780E-03-0.29024817E-06 0.55354910E-10-0.38875822E-14    2
-0.73293478E 05-0.16564590E 02 0.53451571E 01 0.16916668E-01-0.25004302E-04    3
 0.16713939E-07-0.41452878E-11-0.72452431E 05 0.30263715E 01                     4
ALCL3(S)            J 3/64AL  1CL  300  000  0S   300.000   465.600             1
 0.              0.              0.              0.              0.               2
 0.              0.              0.14431409E 02-0.24545071E-01 0.20035127E-04    3
 0.14508072E-06-0.21371474E-09-0.88404228E 05-0.63344384E 02                     4
ALCL3(L)            J 3/64AL  1CL  300  000  0L   465.600  5000.000             1
```

```
 0.13385264E 02 0.              0.              0.              0.               2
-0.84887230E 05-0.54682110E 02 0.13385264E 02 0.              0.               3
 0.              0.             -0.84887230E 05-0.54682110E 02                   4
ALF                 J 9/64AL  1F   100  000  0G   300.000  5000.000              1
 0.41432941E 01 0.43456010E-03-0.16460575E-06 0.30802017E-10-0.21262355E-14      2
-0.32778410E 05 0.19573280E 01 0.28236585E 01 0.48021164E-02-0.53444016E-05      3
 0.24433850E-08-0.28283365E-12-0.32462959E 05 0.85613734E 01                     4
ALF+                J 6/68AL  1F   1E  -10   0G   300.000  5000.000              1
 0.41957106E 01 0.38290900E-03-0.13075649E-06 0.22591321E-10-0.13164857E-14      2
 0.79682722E 05 0.24475601E 01 0.28575830E 01 0.50617403E-02-0.61248583E-05      3
 0.32221582E-08-0.54448503E-12 0.79991210E 05 0.90992312E 01                     4
ALF2                J 9/64AL  1F   200  000  0G   300.000  5000.000              1
 0.61804240E 01 0.90488677E-03-0.38832937E-06 0.73713932E-10-0.51591978E-14      2
-0.85071157E 05-0.39592295E 01 0.33301792E 01 0.10295891E-01-0.11444803E-04      3
 0.51484409E-08-0.56416287E-12-0.84387796E 05 0.10315035E 02                     4
ALF2+               J 6/68AL  1F   2E  -10   0G   300.000  5000.000              1
 0.68767776E 01 0.68899880E-03-0.29551540E-06 0.56021377E-10-0.39146708E-14      2
 0.18916320E 05-0.10625708E 02 0.37787286E 01 0.12332101E-01-0.16840570E-04      3
 0.10394906E-07-0.23427970E-11 0.19590891E 05 0.45427075E 01                     4
ALF2-               J 6/68AL  1F   2F   10   0G   300.000  5000.000              1
 0.61130125E 01 0.97687473E-03-0.41809432E-06 0.79151704E-10-0.55256597E-14      2
-0.90104129E 05-0.46096515E 01 0.30389102E 01 0.11066587E-01-0.12222733E-04      3
 0.54253437E-08-0.56268792E-12-0.89365118E 05 0.10795330E 02                     4
ALF3(S)             J 9/65AL  1F   300  000  0S   300.000   718.000              1
 0.              0.              0.              0.              0.               2
 0.              0.              0.13819544E 01 0.37097544E-01-0.41036006E-04      3
 0.60619212E-08 0.13766618E-10-0.18326806E 06-0.91844203E 01                     4
ALF3(S)             J 9/65AL  1F   300  000  0S   718.000  2500.000              1
 0.10522523E 02 0.20940523E-02-0.45541742E-06 0.19209506E-09-0.29475093E-13      2
-0.18482520E 06-0.52885029E 02 0.46589212E 01 0.15809473E-01 0.71160071E-06      3
-0.20754789E-07 0.11298614E-10-0.18335719E 06-0.22679313E 02                     4
ALF3                J 9/65AL  1F   300  000  0G   300.000  5000.000              1
 0.86545610E 01 0.14919760E-02-0.64334360E-06 0.12269734E-09-0.86255143E-14      2
-0.14863571E 06-0.17064964E 02 0.36893150E 01 0.13583806E-01-0.22267274E-04      3
 0.11536770E-07-0.19253509E-11-0.14747858E 06 0.75283682E 01                     4
ALH                 J 6/63AL  1H   100  000  0G   300.000  5000.000              1
 0.33366898E 01 0.12377864E-02-0.49869941E-06 0.92294633E-10-0.63451694E-14      2
 0.30091761E 05 0.30823232E 01 0.36576857E 01-0.19744698E-02 0.68663398E-05      3
-0.62041404E-08 0.18663103E-11 0.30146458E 05 0.20753460E 01                     4
ALN(S)              J12/62AL  1N   100  000  0S   300.000  3000.000              1
 0.47788460E 01 0.20198156E-02-0.12548670E-05 0.36283351E-09-0.39253241E-13      2
-0.40062784E 05-0.26091961E 02-0.77586359E-01 0.17149061E-01-0.17948725E-04      3
 0.72995522E-08-0.55492557E-12-0.38837399E 05-0.15105473E 01                     4
ALN                 J 3/67AL  1N   100  000  0G   300.000  5000.000              1
 0.40281038E 01 0.56430940E-03-0.22198395E-06 0.42074947E-10-0.29421886E-14      2
 0.51028644E 05 0.21456703E 01 0.28422305E 01 0.39430202E-02-0.32513003E-05      3
 0.58151994E-09 0.29409158E-12 0.51340666E 05 0.83219266E 01                     4
ALO                 J 9/65AL  1O   100  000  0G   300.000  5000.000              1
 0.39717174E 01 0.63262200E-03-0.25846015E-06 0.49488774E-10-0.33027949E-14      2
 0.95752335E 04 0.32492563E 01 0.29297104E 01 0.31210445E-02-0.13586470E-05      3
-0.11939557E-08 0.89331277E-12 0.98709961E 04 0.85935845E 01                     4
ALO+                J 6/68AL  1O   1E  -10   0G   300.000  5000.000              1
 0.89679966E 01-0.29837240E-02 0.66474633E-06-0.33205343E-10 0.27636991E-14      2
 0.11691005E 06-0.27332300E 02 0.52645833E 01-0.14004473E-01 0.38815976E-04      3
-0.28971726E-07 0.55086564E-11 0.11953910E 06-0.15025814E 01                     4
ALOCL               J 9/64AL  1O   1CL  100  0G   300.000  5000.000              1
 0.67305200E 01 0.79662822E-03-0.34233355E-06 0.65922648E-10-0.45519107E-14      2
-0.44030832E 05-0.93132976E 01 0.32444409E 01 0.14117009E-01-0.19722038E-04      3
 0.11962798E-07-0.27099180E-11-0.43312343E 05 0.79922149E 01                     4
ALOF                J 3/64AL  1O   1F   100  0G   300.000  5000.000              1
 0.64257366E 01 0.11920086E-02-0.51432842E-06 0.98028793E-10-0.68852831E-14      2
-0.72744937E 05-0.93298977E 01 0.17646910E 01 0.17378839E-01-0.22537031E-04      3
 0.12468245E-07-0.23392213E-11-0.71691933E 05 0.13697771E 02                     4
ALOH                J12/67AL  1O   1H   10   0G   300.000  5000.000              1
 0.36350674E 01 0.33636822E-02-0.12466244E-05 0.21382205E-09-0.13898319E-13      2
-0.23046105E 05 0.36766915E 01 0.26132211E 01 0.27716894E-02 0.74157830E-05      3
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-0.11354602E-07 0.45569559E-11-0.22586797E 05 0.10062166E 02                4
ALOH+              J12/67AL  10   1H   1F  -1G   300.000  5000.000          1
 0.41624797E 01 0.28687165E-02-0.10416371E-05 0.17575550E-09-0.11271622E-13 2
-0.15314295E 04 0.25596643E 01 0.19486482E 01 0.80052285E-02-0.25070514E-05 3
-0.37733578E-05 0.24506051E-11-0.90847219E 03 0.14141875E 02                4
ALOH-              J12/67AL  10   1H   1E   1G   300.000  5000.000          1
 0.43010718E 01 0.21668503E-02-0.73968645E-06 0.11821055E-09-0.72209341E-14 2
-0.29134095E 05 0.35138246E 01 0.29130204E 01 0.79530715E-02-0.30558054E-05 3
-0.12598709E-08 0.12886094E-11-0.28781827E 05 0.10509284E 02                4
ALO2               J 6/65AL  10   20   00   0G   300.000  5000.000          1
 0.65519349E 01 0.10730596E-02-0.47379153E-06 0.91825185E-10-0.63074266E-14 2
-0.16146809E 03-0.85088553E 01 0.32187326E 01 0.12556176E-01-0.14970696E-04 3
 0.76845277E-08-0.12520185E-11 0.61344440E 03 0.89519547E 01                4
ALO2-              J 6/68AL  10   2E   10   0G   300.000  5000.000          1
 0.62810376E 01 0.13358850E-02-0.57146602E-06 0.10535642E-09-0.75832579E-14 2
-0.23262269E 05-0.86956341E 01 0.32378637E 01 0.10596234E-01-0.10216156E-04 3
 0.34746059E-08 0.53681451E-13-0.22488188E 05 0.67504624E 01                4
ALO2H              J 3/64AL  10   2H   100  0G   300.000  5000.000          1
 0.64270590E 01 0.32216643E-02-0.12130266E-05 0.21051077E-09-0.13807378E-13 2
-0.33973090E 05-0.74745628E 01 0.24468083E 01 0.16385868E-01-0.16625070E-04 3
 0.70661078E-08-0.64131253E-12-0.33025991E 05 0.12433532E 02                4
AL2CL6             J 3/64AL  2CL  600  000  0G   300.000  5000.000          1
 0.20830991E 02 0.13027630E-02-0.56153351E-06 0.10680317E-09-0.74806257E-14 2
-0.16217187E 06-0.62572214E 02 0.12171270E 02 0.36713644E-01-0.55603458E-04 3
 0.38113797E-07-0.97237068E-11-0.16042879E 06-0.20882840E 02                4
AL2O               J 9/65AL  20   100  000  0G   300.000  5000.000          1
 0.61309407E 01 0.96280169E-03-0.41516089E-06 0.79211578E-10-0.55717813E-14 2
-0.17829876E 05-0.44030124E 01 0.34117107E 01 0.95983909E-02-0.10306122E-04 3
 0.42754762E-08-0.32573380E-12-0.17165738E 05 0.92734405E 01                4
AL2O+              J 6/68AL  20   1E  -10   0G   300.000  5000.000          1
 0.61392920E 01 0.94849579E-03-0.40671071E-06 0.77181909E-10-0.54019669E-14 2
 0.71439805E 05-0.40782213E 01 0.33910609E 01 0.95468013E-02-0.10650036E-04 3
 0.46034848E-08-0.43845353E-12 0.72108359E 05 0.97287393E 01                4
AL2O2              J 9/65AL  20   200  000  0G   300.000  5000.000          1
 0.77227053E 01 0.25161623E-02-0.10830293E-05 0.20637292E-09-0.14502168E-13 2
-0.51613928E 05-0.13589237E 02 0.15995687E 01 0.19382190E-01-0.16555045E-04 3
 0.32432492E-08 0.13877467E-11-0.50096135E 05 0.16211774E 02                4
AL2O2+             J 6/68AL  20   2E  -10   0G   300.000  5000.000          1
 0.80829239E 01 0.21259695E-02-0.91683420E-06 0.17488147E-09-0.12295690E-13 2
 0.63056018E 05-0.14431680E 02 0.18140836E 01 0.22238435E-01-0.23492838E-04 3
 0.94504231E-08-0.55539774E-12 0.64583715E 05 0.17091430E 02                4
AL2O3(S)           J 3/64AL  20   300  000  0S   300.000  2315.000          1
 0.12533023E 02 0.26483766E-02-0.11252155E-08-0.25404218E-09 0.50340293E-13 2
-0.20591407E 06-0.67517363E 02-0.25071773E 01 0.62271160E-01-0.89940804E-04 3
 0.60690359E-07-0.15530958E-10-0.20281921E 06 0.53456899E 01                4
AL2O3(L)           J 3/64AL  20   300  000  0L  2315.000  5000.000          1
 0.17422481E 02 0.              0.             0.             0.            2
-0.19704127E 06-0.93759984E 02 0.              0.             0.            3
 0.             0.              0.             0.                           4
AR                 L 5/66AR  100  000  000  0G   300.000  5000.000          1
 0.25000000E 01 0.              0.             0.             0.            2
-0.74537502E 03 0.43660006E 01 0.25000000E 01 0.             0.            3
 0.             0.             -0.74537498E 03 0.43660006E 01               4
AR+                L12/66AR  1E  -100  000  0G   300.000  5000.000          1
 0.28420672E 01-0.37648603E-04-0.26463209E-07 0.12240311E-10-0.11885139E-14 2
 0.18272563E 06 0.36720201E 01 0.24857001E 01-0.55682660E-03 0.33194849E-05 3
-0.39236795E-08 0.14143279E-11 0.18290215E 06 0.53380154E 01                4
B(S)               J12/64B   10   00   00   0S   300.000  2450.000          1
 0.21353847E 01 0.62284826E-03 0.52269843E-06-0.34412816E-09 0.54070294E-13 2
-0.87167211E 03-0.12048934E 02-0.13181931E 01 0.11950484E-01-0.10999163E-04 3
 0.21567584E-08 0.12019863E-11-0.45597194E 02 0.51212201E 01                4
B(L)               J12/64B   10   00   00   0L  2450.000  5000.000          1
 0.35739752E 01 0.              0.             0.             0.            2
 0.41164170E 03-0.21048345E 02 0.              0.             0.            3
 0.             0.              0.             0.                           4
B                  J12/64B   100  000  000  0G   300.000  5000.000          1
```

```
 0.25124741E 01-0.25820555E-04 0.18396008E-07-0.55496146E-11 0.61569370E-15    2
 0.66076153E 05 0.41307263F 01 0.25022979E 01-0.91340917E-06-0.15435319E-07    3
 0.26217528E-10-0.12045083E-13 0.66079744E 05 0.41856076E 01                   4
B+               J12/67B   1E   -10   00   0G   300.000  5000.000              1
 0.25106353E 01-0.22902600E-04 0.16805879E-07-0.50849164E-11 0.54628543E-15    2
 0.16233962E 06 0.23484087E 01 0.24991667E 01 0.55246273E-05-0.12821246F-07    3
 0.12516710E-10-0.43867904E-14 0.16234334E 06 0.24093838E 01                   4
BCL              J12/64B   1CL  100  000   0G   300.000  5000.000              1
 0.41020571F 01 0.48655193E-03-0.19864326E-06 0.35933242E-10-0.25099069E-14    2
 0.15687958E 05 0.19420655E 01 0.28364463E 01 0.44368817E-02-0.43887522E-05    3
 0.15161078E-08 0.32646195E-13 0.16001361E 05 0.83321464E 01                   4
BCL+             J 6/68B   1CL  1E   -10   0G   300.000  5000.000              1
 0.41060888E 01 0.47274170E-03-0.17928584E-06 0.32416137E-10-0.20545759F-14    2
 0.14713097E 06 0.26295615E 01 0.28124197E 01 0.45006392E-02-0.45119962E-05    3
 0.19672216E-08-0.13837802E-12 0.14744849E 06 0.91435145E 01                   4
BCLF             J12/64B   1CL  1F   100   0G   300.000  5000.000              1
 0.57076757E 01 0.14100203E-02-0.60114137E-06 0.11367044E-09-0.79368063E-14    2
-0.39693327E 05-0.15482176E 01 0.33120234E 01 0.74198763E-02-0.43485949E-05    3
-0.11374057E-08 0.13763890E-11-0.39017548E 05 0.10935177E 02                   4
BCL2             J12/64B   1CL  200  000   0G   300.000  5000.000              1
 0.61443257E 01 0.94438848E-03-0.40551078E-06 0.77051714E-10-0.53930787E-14    2
-0.12097450E 05-0.29714082E 01 0.33541925E 01 0.93759716E-02-0.10655452E-04    3
 0.45615910E-08-0.41141656E-12-0.11426382E 05 0.10854976E 02                   4
BCL2+            J 6/68B   1CL  2E   -10   0G   300.000  5000.000              1
 0.69266627E 01 0.67777633E-03-0.32101496F-06 0.68344422F-10-0.50073592E-14    2
 0.72265517E 05-0.89477869E 01 0.42704931E 01 0.10603791E-01-0.14229838E-04    3
 0.85372831E-08-0.18349671E-11 0.72843711F 05 0.40632904E 01                   4
BCL2-            J 6/68B   1CL  2E   10    0G   300.000  5000.000              1
 0.35371621E 01 0.55331412E-02-0.24172338E-05 0.43033015E-09-0.27509819E-13    2
-0.23769006E 05 0.10676847E 02 0.32768955E 01 0.10605370E-01-0.12996034E-04    3
 0.74902370E-08-0.13205279F-11-0.29024943E 05 0.10561853E 02                   4
BCL3             J12/64B   1CL  300  000   0G   300.000  5000.000              1
 0.85989538OF 01 0.15531923E-02-0.67000602E-06 0.12789112E-09-0.90003059E-14   2
-0.51357071E 05-0.15171594E 02 0.37395265E 01 0.18105813E-01-0.21348461E-04    3
 0.10828335E-07-0.17325967E-11-0.50214609E 05 0.90399632E 01                   4
BF               J12/64B   1F   100  000   0G   300.000  5000.000              1
 0.35771838E 01 0.10192903F-02-0.41251564E-06 0.77196438E-10-0.53498741F-14    2
-0.15127264E 05 0.32529083F 01 0.34613609E 01-0.95685468E-03 0.60135744E-05    3
-0.64978057E-08 0.22355349E-11-0.14969820E 05 0.44475660E 01                   4
BF2              J12/64B   1F   200  000   0G   300.000  5000.000              1
 0.52460775F 01 0.18901144E-02-0.80019689E-06 0.15067869E-09-0.10493457F-13    2
-0.67259288E 05-0.11928535E 01 0.34562272E 01 0.47109600E-02 0.10919029E-05    3
-0.52261995E-08 0.24432391F-11-0.66657099F 05 0.35323412E 01                   4
BF2+             J 6/68B   1F   2E   -10   0G   300.000  5000.000              1
 0.58127638E 01 0.18193424E-02-0.77103457F-06 0.14489732E-09-0.99809157E-14    2
 0.40267034E 05-0.70174886F 01 0.33146474E 01 0.36443654F-02-0.67525396E-05    3
 0.13383665E-08 0.45114910E-12 0.40955931E 05 0.58915131E 01                   4
BF2-             J 6/68B   1F   2E   10    0G   300.000  5000.000              1
 0.57561208E 01 0.56712487E-03 0.51635707E-06-0.21643437E-09 0.21208230F-13    2
-0.82440186E 05-0.44932833E 01 0.25987348E 01 0.97441257E-02-0.70812555E-05    3
-0.53370797E-10 0.14368424F-11-0.81662465F 05 0.11530975E 02                   4
BF3              J 9/65B   1F   300  000   0G   300.000  5000.000              1
 0.70329976E 01 0.32052480E-02-0.13599556E-05 0.25657976E-09-0.17899026E-13    2
-0.13929312E 06-0.11273589E 02 0.24373484F 01 0.15344154E-01-0.10953116E-04    3
 0.86431529E-09 0.14242375E-11-0.13800960E 06 0.12586370E 02                   4
BH               J12/64B   1H   100  000   0G   300.000  5000.000              1
 0.28919079E 01 0.15832546F-02-0.53261729E-06 0.10242068E-09-0.67669569E-14    2
 0.52328714E 05 0.37829483E 01 0.36862206E 01-0.13055435E-02 0.26742105E-05    3
-0.91073739E-09-0.15591136F-12 0.52176339E 05-0.68540385E-01                   4
BHF2             J12/65B   1H   1F   200   0G   300.000  5000.000              1
 0.53164527E 01 0.47444466E-02-0.19337858F-05 0.35583392F-09-0.24293667E-13    2
-0.90375012E 05-0.30563344E 01 0.24053602E 01 0.92755844E-02 0.13386461E-05    3
-0.86807895E-08 0.41211015E-11-0.89388409E 05 0.12874850E 02                   4
BH2              J12/64B   1H   200  000   0G   300.0     5000.000              1
 0.33625285E 01 0.39012854E-02-0.15097551E-05 0.26672   E-09-0.17713053F-13    2
 0.22313028E 05 0.12459933E 01 0.23958282E 01 0.74776260E-02-0.72019514E-05    3
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 0.45826398E-08-0.12510680E-11 0.23162650E 05 0.60631811E 01                   4
BH3                 J12/64B  1H   300  000  0G   300.000  5000.000             1
 0.20621726E 01 0.72655895E-02-0.27510337E-05 0.47303709E-09-0.31334255E-13    2
 0.11923753E 05 0.88361664E 01 0.39487033E 01-0.52170543E-03 0.76481164E-05    3
-0.46148694E-08 0.56318616E-12 0.11618809E 05-0.58801582E-01                   4
BN(S)               J 6/66B  1N   100  000  0S   300.000  3500.000             1
 0.90909293E 00 0.81143277E-02-0.48032086E-05 0.12291916E-08-0.11517125E-12    2
-0.30855565E 05-0.58284489E 01-0.11182452E 01 0.15038275E-01-0.11557560E-04    3
 0.21058502E-08 0.11962119E-11-0.30413091E 05 0.41742190E 01                   4
BN                  J 6/66B  1N   100  000  0G   300.000  5000.000             1
 0.35931532E 01 0.37176305E-03-0.29972644E-06 0.56036944E-10-0.40750421E-14    2
 0.56171241E 05 0.45869994E 01 0.35375065E 01-0.13566586E-02 0.62214189E-05    3
-0.61683259E-08 0.19872461E-11 0.56329743E 05 0.55499509E 01                   4
BO                  J 6/66B  10   10   00   0G   300.000  5000.000             1
 0.31564956E 01 0.13816589E-02-0.[illegible]5049630E-06 0.93116678E-10-0.64164546E-14    2
-0.10303422E 04 0.60242706E 01 0.37297250E 01-0.20375324E-02 0.57362549E-05    3
-0.43894828E-08 0.10916632E-11-0.10618859E 04 0.36123221E 01                   4
BOCL                J 3/65B  10   1CL  100  0G   300.000  5000.000             1
 0.57135566E 01 0.13664689E-02-0.77487898E-06 0.14398572E-09-0.99317745E-14    2
-0.39977353E 05-0.48935834E 01 0.32705321E 01 0.10227750E-01-0.12070163E-04    3
 0.72025562E-08-0.16914738E-11-0.39373208E 05 0.73361224E 01                   4
BOF                 J 3/65B  10   1F   100  0G   300.000  5000.000             1
 0.52618488E 01 0.23462431E-02-0.97620810E-06 0.18167625E-09-0.12545891E-13    2
-0.74324949E 05-0.40691029E 01 0.27741495E 01 0.93927631E-02-0.79998507E-05    3
 0.27457058E-08-0.11175219E-12-0.73640460E 05 0.37507490E 01                   4
BOF2                J12/66B  10   1F   200  0G   300.000  5000.000             1
 0.73077233E 01 0.29903620E-02-0.13059617E-05 0.25308242E-09-0.17687333E-13    2
-0.10334576E 06-0.11205602E 02 0.17445977E 01 0.18693277E-01-0.15246164E-04    3
 0.26559470E-08 0.13798806E-11-0.10186759E 06 0.17339953E 02                   4
BO2                 J 6/66B  10   20   00   0G   300.000  5000.000             1
 0.53198434E 01 0.18626574E-02-0.81302797E-06 0.15735821E-09-0.10944238E-13    2
-0.36255117E 05-0.65741060E 01 0.31212049E 01 0.84680883E-02-0.45972278E-05    3
-0.16420021E-08 0.16658233E-11-0.35483307E 05 0.75346936E 01                   4
BO2-                J 6/66B  10   2E   10   0G   300.000  5000.000             1
 0.48805169E 01 0.26743651E-02-0.10932194E-05 0.20020673E-09-0.13717769E-13    2
-0.61632539E 05-0.30224936E 01 0.24916337E 01 0.97470644E-02-0.87640864E-05    3
 0.35502544E-08-0.40611221E-12-0.60939433E 05 0.92136795E 01                   4
BS                  J 3/65B  1S   100  000  0G   300.000  5000.000             1
 0.37891419E 01 0.79620103E-03-0.32499623E-06 0.61086740E-10-0.42442958E-14    2
 0.39005219E 05 0.39725230E 01 0.31819722E 01 0.93156211E-03 0.29013321E-05    3
-0.45074902E-08 0.18098145E-11 0.39248590E 05 0.74975225E 01                   4
B2                  J12/64B  200  000  000  0G   300.000  5000.000             1
 0.39119970E 01 0.69145978E-03-0.27146628E-06 0.51110013E-10-0.35535897E-14    2
 0.96841827E 05 0.15798824E 01 0.29873313E 01 0.24872377E-02-0.94106611E-07    3
-0.21303174E-08 0.11299017E-11 0.97128274E 05 0.65267343E 01                   4
B2C                 J 6/66B  20   100  000  0G   300.000  5000.000             1
 0.47300538E 01 0.23941486E-02-0.10008324E-05 0.18697510E-09-0.12953672E-13    2
 0.98853354E 04-0.64909402E 00 0.35294730E 01 0.31993226E-02 0.30329257E-05    3
-0.57491255E-08 0.22847349E-11 0.10363201E 05 0.62263887E 01                   4
B2O2                J12/64B  20   200  000  0G   300.000  5000.000             1
 0.69938574E 01 0.35940393E-02-0.14753611E-05 0.27225124E-09-0.18695996E-13    2
-0.57236178E 05-0.12180936E 02 0.35807078E 01 0.15361132E-01-0.18606397E-04    3
 0.12171451E-07-0.32411018E-11-0.56486647E 05 0.43429084E 01                   4
B2O3(L)             J12/64B  20   300  000  0L   300.000  5000.000             1
 0.18425107E 02-0.44082357E-02 0.22150768E-05-0.45762510E-09 0.35327399E-13    2
-0.15506558E 06-0.99478274E 02 0.28551333E 02-0.17943221E 00 0.50520348E-03    3
-0.52179873E-06 0.18327671E-09-0.15465810E 06-0.11793083E 03                   4
B2O3                J12/64B  20   300  000  0G   300.000  5000.000             1
 0.84015760E 01 0.47392003E-02-0.19523814E-05 0.36115921E-09-0.24845211E-13    2
-0.10323545E 06-0.15835109E 02 0.36780431E 01 0.20138386E-01-0.21637125E-04    3
 0.11927398E-07-0.25819915E-11-0.10203007E 06 0.80209606E 01                   4
B3O3CL3             J 3/65B  30   3CL  300  0G   300.000  5000.000             1
 0.19287564E 02 0.63172531E-02-0.27242926E-05 0.52047910E-09-0.36677790E-13    2
-0.20320883E 06-0.67898332E 02 0.40444983E 01 0.54260597E-01-0.55750761E-04    3
 0.22223128E-07-0.14181295E-11-0.19941632E 06 0.90435427E 01                   4
B3O3F3              J 3/65B  30   3F   300  0G   300.000  5000.000             1
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 0.16658616E 02 0.89685754E-02-0.37881058E-05 0.71370401E-09-0.50376917E-13   2
-0.29093104E 06-0.59871948E 02 0.30798861F 01 0.45636592F-01-0.33093926E-04   3
 0.25536839E-08 0.44358761E-11-0.28712213E 06 0.11462195E 02                  4
BE(S)              J 9/61BE  10    00    00   0S   300.000  1556.000          1
 0.16336257E 01 0.13981070F-02-0.51915094F-03-0.40357551E-09 0.15576542E-12   2
-0.54430376E 03-0.87156145E 01-0.53886197E 00 0.13250958E-01-0.19860267E-04   3
 0.13938457E-07-0.35115543E-11-0.27818237E 03 0.10351100E 01                  4
BE(L)              J 9/61BE  10    00    00   0L  1556.000  5000.000          1
 0.31549997E 01-0.46473346E-04 0.27783586F-06-0.83431677E-10 0.81533123E-14   2
 0.30546750E 03-0.16456535E 02 0.              0.              0.             3
 0.             0.             0.              0.                             4
BE                 J 9/61BE  100   000   000  0G   300.000  5000.000          1
 0.24060350E 01 0.13872751E-03-0.1 913206E-06 0.24973727E-10-0.56423640E-15   2
 0.38656155E 05 0.26445402E 01 0.24982460E 01 0.12910008E-04-0.33182303E-07   3
 0.35564329E-10-0.13528107E-13 0.38633140E 05 0.21401114E 01                  4
BE+                J 6/65BE  1E   -100   000  0G   300.000  5000.000          1
 0.25101862E 01-0.21688740F-04 0.15756684E-07-0.47788232E-11 0.52465496E-15   2
 0.14754576E 06 0.27707490E 01 0.24942733E 01 0.41392101E-04-0.10472877E-06   3
 0.11080231F-09-0.41739398E-13 0.14754985E 06 0.28498691E 01                  4
BEBO2              J 6/66BE  1B    10    200  0G   300.000  5000.000          1
 0.69108376E 01 0.32668684E-02-0.13673120F-05 0.25576211E-09-0.17727741E-13   2
-0.60505715E 05-0.91748501E 01 0.20069120E 01 0.18044824E-01-0.16917581E-04   3
 0.60865373E-08-0.17276285E-12-0.59234197E 05 0.15792365E 02                  4
BECL               J 9/66BE  1CL   100   000  0G   300.000  5000.000          1
 0.41052878E 01 0.47461701E-03-0.17996528E-06 0.32563903E-10-0.20652840F-14   2
 0.59753060E 04 0.24513644E 01 0.28321987E 01 0.44566764E-02-0.44482161E-05   3
 0.17852587E-06 0.45206894E-14 0.62905248E 04 0.85784075E 01                  4
BECL+              J 6/68BE  1CL   1E   -10   0G   300.000  5000.000          1
 0.53827500E 01-0.18471198E-02 0.11123683E-05-0.16952994E-09 0.61007091E-14   2
 0.11599717E 06-0.50753759E 01 0.28965984E 01 0.51287482E-02-0.64427911E-05   3
 0.35632640E-08-0.65925039E-12 0.11671486E 06 0.73241359E 01                  4
BECLF              J 6/65BE  1CL   1F    100  0G   300.000  5000.000          1
 0.64402731E 01 0.11463693E-02-0.48545360E-06 0.91287865E-10-0.63443549E-14   2
-0.71059771E 05-0.77418556E 01 0.41024381E 01 0.85017490E-02 0.89093963E-05   3
 0.40076232E-08-0.51627539E-12-0.70468736E 05 0.40860069E 01                  4
BECL2(S)           J 6/65BE  1CL   200   000  0S   300.000   695.000          1
 0.             0.             0.              0.              0.             2
 0.             0.             0.30065745E 01 0.19539559E-01-0.48913605E-05   3
-0.29604159F-07 0.23534561E-10-0.64722100F 05-0.12579772E 02                  4
BECL2(L)           J 6/65BE  1CL   200   000  0L   695.000  5000.000          1
 0.14603719E 02 0.             0.              0.              0.             2
-0.64498417E 05-0.76448784E 02 0.14603719E 02 0.              0.             3
 0.             0.            -0.64498417E 05-0.76448784E 02                  4
BECL2              J 6/65BE  1CL   200   000  0G   300.000  5000.000          1
 0.67043191E 01 0.87164463E-03-0.37255053E-06 0.70567006E-10-0.49335360E-14   2
-0.45494558F 05-0.86351641E 01 0.44927125E 01 0.60535545E-02-0.85319239F-05   3
 0.40397049E-08-0.53498092E-12-0.44952881E 05 0.26826695E 01                  4
BEF                J 3/63BE  1F    100   000  0G   300.000  5000.000          1
 0.37145220E 01 0.38444143E-03-0.35713612E-06 0.67097461E-10-0.46621539F-14   2
-0.26229052E 05 0.31239768E 01 0.37725419E 01 0.23049431E-03 0.40167391E-05   3
-0.52234254F-08 0.19829320F-11-0.26012685E 05 0.53573716F 01                  4
BEF2(S)            J 6/64BE  1F    200   000  0S   300.000   815.000          1
 0.             0.             0.              0.              0.             2
 0.             0.            -0.50845988F 01 0.60246397E-01-0.81938471E-04   3
 0.17432430E-07 0.23140642E-10-0.12239759E 06 0.20892532E 02                  4
BEF2(L)            J 5/64BE  1F    200   000  0L   815.000  5000.000          1
 0.10567314E 02 0.             0.              0.              0.             2
-0.12533992E 06-0.55211844E 02 0.10567314F 02 0.              0.             3
 0.             0.            -0.12533992E 06-0.55211844F 02                  4
BEF2               J 6/64BE  1F    200   000  0G   300.000  5000.000          1
 0.60675072F 01 0.19325223F-02-0.84526125E-06 0.17696872E-09-0.83933147E-14   2
-0.96391008F 05-0.78701494E 01 0.35843833F 01 0.93243776F-02-0.88131513F-05   3
 0.38779196E-08-0.50612451F-12-0.95770860F 05 0.42561107E 01                  4
BEH                J 3/63BE  1H    100   000  0G   300.000  5000.000          1
 0.30570218E 01 0.14977223E-02-0.56872963E-06 0.10260317E-09-0.69166979F-14   2
 0.37639513E 05 0.33273052E 01 0.37312305E 01-0.19142548E-02 0.48910325E-05   3
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-0.32925853E-08 0.66628562E-12 0.37565563E 05 0.37543895E 00                   4
BEH+                J 9/66BE  1H   1E  -100  0G   300.000  5000.000            1
 0.29015992E 01 0.16751761E-02-0.66805507E-06 0.12510951E-09-0.81741466E-14    2
 0.17816812E 06 0.35425415E 01 0.37095712E 01-0.15852031E-02 0.36225769E-05    3
-0.18933221E-08 0.17173264E-12 0.13302866E 06-0.29598407E 00                   4
BEN                 J 6/63BE  1N   100  000  0G   300.000  5000.000            1
 0.37855937E 01 0.92286575E-03-0.32711602E-06 0.61551824E-10-0.42609041E-14    2
 0.50056180E 05 0.30924194E 01 0.31684286E 01 0.10782498E-02 0.27376017E-05    3
-0.43481099E-08 0.17534453E-11 0.50310451E 05 0.66493591E 01                   4
BEO(S)              J 9/63BE  10   100  000  0S   300.000  2820.000            1
 0.33180450E 01 0.55917212E-02-0.46301271E-05 0.13108779E-08-0.27843047E-12    2
-0.73451553E 05-0.19304223E 02-0.19723349E 01 0.24764354E-01-0.31498330E-0     3
 0.19540031E-07-0.49216319E-11-0.72270069E 05 0.67863119E 01                   4
BEO(L)              J 9/63BE  10   100  000  0L  2820.000  5000.000            1
 0.80512867E 01 0.             0.             0.             0.                2
-0.71298168E 05-0.46972346E 02 0.             0.             0.                3
 0.             0.             0.             0.                               4
BEO                 J 9/63BE  10   100  000  0G   300.000  5000.000            1
 0.35048549E 01 0.10867884E-02-0.43930877E-06 0.82088967E-10-0.56778800E-14    2
 0.14435010E 05 0.33167347E 01 0.35250620E 01-0.13044281E-02 0.62838237E-05    3
-0.63674976E-08 0.20911849E-11 0.14562192E 05 0.38321456E 01                   4
BEOH                J 9/63BE  10   1H   100  0G   300.000  5000.000            1
 0.36351960E 01 0.28532436E-02-0.10230326E-05 0.17069994E-09-0.10840994E-13    2
-0.13856067E 05 0.51296294E 01 0.37270356E 01-0.34554824E-03 0.82188520E-05    3
-0.92269046E-08 0.32518302E-11-0.13732272E 05 0.53399404E 01                   4
BEOH+               J 6/68BE  10   1H   1F  -1G   300.000  5000.000            1
 0.37549335E 01 0.33439583E-02-0.12505263E-05 0.21596827E-09-0.14114778E-13    2
 0.96194409E 05 0.14057049E 01 0.24619220E 01 0.36977984E-02 0.59446561E-05    3
-0.10392932E-07 0.43387733E-11 0.96693753E 05 0.88341583E 01                   4
BEO2H2              J 3/67BE  10   2H   200  0G   300.000  5000.000            1
 0.64853231E 01 0.58388339E-02-0.21839203E-05 0.37665248E-09-0.24568934E-13    2
-0.81124230E 05-0.93680114E 01 0.24681022E 01 0.13712514E-01-0.16655536E-04    3
 0.62752158E-08-0.30697537E-12-0.80137138E 05 0.10955417E 02                   4
BE2O                J 9/63BE  20   100  000  0G   300.000  5000.000            1
 0.54549734E 01 0.21970385E-02-0.92919578E-06 0.17496410E-09-0.12189982E-13    2
-0.94958985E 04-0.56235860E 01 0.27527897E 01 0.89648699E-02-0.55359247E-05    3
-0.34769188E-09 0.11015472E-11-0.87174709E 04 0.84387556E 01                   4
BE2OF2              J 6/66BE  20   1F   200  0G   300.000  5000.000            1
 0.10311343E 02 0.29258151E-02-0.12481987E-05 0.23652169E-09-0.16559160E-13    2
-0.14844623E 06-0.24500846E 02 0.48600026E 01 0.19438982E-01-0.18818760E-04    3
 0.71009503E-08-0.37225258E-12-0.14703959E 06 0.32285704E 01                   4
BE2O2               J 9/63BE  20   200  000  0G   300.000  5000.000            1
 0.71783552E 01 0.30798926E-02-0.13162273E-05 0.24970614E-09-0.17496339E-13    2
-0.51934876E 05-0.12938758E 02 0.17102739E 01 0.18244939E-01-0.14377253E-04    3
 0.21268816E-08 0.14691993E-11-0.50512366E 05 0.15201347E 02                   4
BE3O3               J 9/63BE  30   300  000  0G   300.000  5000.000            1
 0.91907322E 01 0.73623701E-02-0.31292729E-05 0.59162589E-09-0.41360194E-13    2
-0.13631849E 06-0.23330943E 02 0.20002692E 01 0.29005172E-01 0.57517847E-06    3
-0.17092805E-07 0.84862785E-11-0.12826867E 06 0.15607790E 02                   4
BE4O4               J 9/63BE  40   400  000  0G   300.000  5000.000            1
 0.14547030E 02 0.91903730E-02-0.35162759E-05 0.66923457E-09-0.47005963E-13    2
-0.19704845E 06-0.51509929E 02-0.13813438E 01 0.52348828E-01-0.40893018E-04    3
 0.47379707E-08 0.49954164E-11-0.19278356E 06 0.39399903E 02                   4
C(S)                J 3/61C   10   00   00   0S   300.000  5000.000            1
 0.13604942E 01 0.19182237E-02-0.84040389E-06 0.16448707E-09-0.11672670E-13    2
-0.55713870E 03-0.80070207E 01-0.44773053E 00 0.53691002E-02-0.39775571E-06    3
-0.40459298E-08 0.21134939E-11-0.94280686E 02 0.16840791E 01                   4
C                   J 3/61C   100  000  000  0G   300.000  5000.000            1
 0.25310663E 01-0.14696202E-03 0.74388084E-07-0.79461079E-11 0.58900977E-16    2
 0.85215294E 05 0.43128879E 01 0.25329705E 01-0.15987641E-03 0.30682082E-06    3
-0.26770064E-09 0.87428827E-13 0.85240422E 05 0.45062374E 01                   4
C+                  L12/66C   1E  -100  000  0G   300.000  5000.000            1
 0.25118274E 01-0.17359784E-04 0.95042676E-08-0.22188518E-11 0.18621892E-15    2
 0.21657721E 06 0.42861293E 01 0.25953840E 01-0.40688649E-03 0.63923669E-06    3
-0.52654878E-09 0.15083377E-12 0.21666281E 06 0.34957298E 01                   4
C-                  J 9/65C   1E   100  000  0G   300.000  5000.000            1
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 0.24470591E 01 0.11286428E-03-0.78591462E-07 0.19778614E-10-0.11105555E-14    2
 0.64977296E 05 0.42356992E 01 0.24925640E 01 0.53153068E-04-0.13307994E-06    3
 0.13951379E-09-0.52150992E-13 0.69955757E 05 0.39811657E 01                   4
CCL               J 3/61C   1CL  100  000  0G   300.000  5000.000              1
 0.41416863E 01 0.40539002E-03-0.16439027E-06 0.30720269E-10-0.21188745E-14    2
 0.65103661E 05 0.31912321E 01 0.32157680E 01 0.28535798E-02-0.18566418E-05    3
-0.34501102E-09 0.54359252E-12 0.65354358E 05 0.79740016E 01                   4
CCL2              J 3/65C   1CL  200  000  0G   300.000  5000.000              1
 0.61038747E 01 0.98444553E-03-0.42074189E-06 0.79586589E-10-0.55531496E-14    2
 0.35712188E 05-0.34096661E 01 0.33799227E 01 0.94958893E-02-0.95663552E-05    3
 0.34526893E-08-0.20537433E-13 0.36333677E 05 0.10347469E 02                   4
CCL3              J12/67C   1CL  30   00   0G   300.000  5000.000              1
 0.89058150E 01 0.12216951E-02-0.52931166E-06 0.10131824E-09-0.71437484E-14    2
 0.64579494E 04-0.15547647E 02 0.33933250E 01 0.21959101E-01-0.30090668E-04    3
 0.18562205E-07-0.41715884E-11 0.76531895E 04 0.11422041E 02                   4
CCL4              J 3/61C   1CL  400  000  0G   300.000  5000.000              1
 0.11545200E 02 0.16301810E-02-0.70898111E-06 0.13620159E-09-0.96350049E-14    2
-0.16836475E 05-0.29758962E 02 0.43356351E 01 0.23628116E-01-0.38939929E-04    3
 0.23746091E-07-0.52279342E-11-0.15320039E 05 0.55306979E 01                   4
CF                J12/67C   1F   10   00   0G   300.000  5000.000              1
 0.36869679E 01 0.91143491E-03-0.36463855E-06 0.67492854E-10-0.45269596E-14    2
 0.28471666E 05 0.41513468E 01 0.34655143E 01-0.68779805E-03 0.56784765E-05    3
-0.64582987E-08 0.22988248E-11 0.28649139E 05 0.53621916E 01                   4
CF2               J 9/66C   1F   200  000  0G   300.000  5000.000              1
 0.52340198E 01 0.20719887E-02-0.95345488E-06 0.21097379E-09-0.15689839E-13    2
-0.22500895E 05-0.19695061E 01 0.27241917E 01 0.74980441E-02-0.21605763E-05    3
-0.40265153E-05 0.24826929E-11-0.21752025E 05 0.11318178E 02                   4
CF3               J 9/64C   1F   300  000  0G   300.000  5000.000              1
 0.71580200E 01 0.30960154E-02-0.13231685E-05 0.25123920E-09-0.17625389E-13    2
-0.60854305E 05-0.11141522E 02 0.23610822E 01 0.15959621E-01-0.11811474E-04    3
 0.11443435E-08 0.14709076E-11-0.59534051E 05 0.13665263E 02                   4
CF4               J 9/64C   1F   400  000  0G   300.000  5000.000              1
 0.91592519E 01 0.42083641E-02-0.18038873E-05 0.34302737E-09-0.24082193E-13    2
-0.11442802E 06-0.23264057E 02 0.11839609E 01 0.27053319E-01-0.23009336E-04    3
 0.52469959E-08 0.14077342E-11-0.11231908E 06 0.17592463E 02                   4
CH                J12/67C   1H   10   00   0G   300.000  5000.000              1
 0.22673116E 01 0.22043000E-02-0.62250191E-06 0.69689940E-10-0.21274952E-14    2
 0.70338037E 05 0.87829352E 01 0.35632752E 01-0.20031372E-03-0.40129814E-06    3
 0.18226922E-08-0.86758311E-12 0.70405506E 05 0.17628023E 01                   4
CH2               J12/62C   1H   200  000  0G   300.000  5000.000              1
 0.27710460E 01 0.40693659E-02-0.14683470E-05 0.24552095E-09-0.15593090E-13    2
 0.46787215E 05 0.47848808E 01 0.28850905E 01 0.36051519E-02 0.79977197E-06    3
-0.27242167E-08 0.12361959E-11 0.46841314E 05 0.53857601E 01                   4
CH3               J12/62C   1H   300  000  0G   300.000  5000.000              1
 0.26916871E 01 0.68035521E-02-0.26088477E-05 0.45775393E-09-0.30236995E-13    2
 0.14915942E 05 0.58225816E 01 0.33479838E 01 0.19900241E-02 0.64982411E-05    3
-0.63603524E-08 0.17971111E-11 0.14925320E 05 0.30286042E 01                   4
CH4               J 3/61C   1H   400  000  0G   300.000  5000.000              1
 0.15027072E 01 0.10416798E-01-0.39181522E-05 0.67777839E-09-0.44283706E-13    2
-0.99737073E 04 0.10707143E 02 0.33261932E 01-0.39794581E-02 0.24558340E-04    3
-0.22732926E-07 0.69626957E-11-0.10144950E 05 0.86690073E 00                   4
CN                J12/66C   1N   100  000  0G   300.000  5000.000              1
 0.36050794E 01 0.73345861E-03 0.14255732E-06-0.16970505E-10-0.30100883E-15    2
 0.54681625E 05 0.35369408E 01 0.37313064E 01-0.18635137E-02 0.45586474E-05    3
-0.29592229E-08 0.56060533E-12 0.54794152E 05 0.34791073E 01                   4
CN-               L 3/67C   1N   1F   100  0G   300.000  5000.000              1
 0.29314417E 01 0.14942618E-02-0.58261650E-06 0.10444145E-09-0.70091727E-14    2
 0.32277395E 04 0.62544561E 01 0.35984234E 01-0.15269918E-02 0.34408627E-05    3
-0.17437245E-08 0.12144973E-12 0.31164996E 04 0.28956093E 01                   4
CN2               J 6/66C   1N   200  000  0G   300.000  5000.000              1
 0.48209077E 01 0.24790014E-02-0.94644109E-06 0.16548764E-09-0.10899129E-13    2
 0.68685948E 05-0.48484039E 00 0.35077779E 01 0.72023958E-02-0.75574589E-05    3
 0.42979217E-08-0.94297935E-12 0.68994281E 05 0.60274964E 01                   4
CO                J 9/65C   1O   100  000  0G   300.000  5000.000              1
 0.29840696E 01 0.14891390E-02-0.57899684E-06 0.10364577E-09-0.69353550E-14    2
-0.14245228E 05 0.63479156E 01 0.37100928E 01-0.16190964E-02 0.36923594E-05    3
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-0.20319674E-08 0.23953344E-12-0.14356310E 05 0.23555351E 01                   4
CCCL                    J12/65C   10   1CL  100  0G   300.000  5000.000        1
 0.54291236E 01 0.16121535E-02-0.66006280E-06 0.12127114E-09-0.82858601E-14    2
-0.93305007E 04 0.36971816E 00 0.42863793E 01 0.50868980E-02-0.50729411E-05    3
 0.29647953E-08-0.77093453E-12-0.90125212E 04 0.62380308E 01                   4
COCL2                   J 6/61C   10   1CL  200  0G   300.000  5000.000        1
 0.77318082E 01 0.24089287E-02-0.10111133E-05 0.18936214E-09-0.13139356E-13    2
-0.29136566E 05-0.11221674E 02 0.31156139E 01 0.13478674E-01-0.22420544E-04    3
 0.12868184E-07-0.27360865E-11-0.28043884E 05 0.11755293E 02                   4
CCF                     J12/65C   10   1F   100  0G   300.000  5000.000        1
 0.48998214E 01 0.22179703E-02-0.92550725E-06 0.17270120E-09-0.11955343E-13    2
-0.22357984E 05 0.97962087E 00 0.32019727E 01 0.55837770E-02-0.14905481E-05    3
-0.23126069E-08 0.13614353E-11-0.21817043E 05 0.10047575E 02                   4
CCF2                    J 3/65C   10   1F   200  0G   300.000  5000.000        1
 0.65651527E 01 0.36511407E-02-0.15332311E-05 0.23720943E-09-0.19930265E-13    2
-0.78818912E 05-0.81745228E 01 0.17992182E 01 0.16576827E-01-0.12529893E-04    3
 0.19894624E-08 0.11147281E-11-0.77502762E 05 0.16463950E 02                   4
COS                     J 3/61C   10   1S   100  0G   300.000  5000.000        1
 0.52392000E 01 0.24100584E-02-0.96064522E-06 0.17778347E-09-0.12235704E-13    2
-0.18480455E 05-0.30910517E 01 0.24625321E 01 0.11947992E-01-0.13794370E-04    3
 0.80707736E-08-0.18327653E-11-0.17803987E 05 0.10792556E 02                   4
CO2                     J 9/65C   10   200  000  0G   300.000  5000.000        1
 0.44608041E 01 0.30981719E-02-0.12392571E-05 0.22741325E-09-0.15525954E-13    2
-0.48961442E 05-0.98635982E 00 0.24007797E 01 0.87350957E-02-0.66070878E-05    3
 0.20021861E-08 0.63274039E-15-0.48377527E 05 0.96951457E 01                   4
CO2-                    J12/66C   10   2E   100  0G   300.000  5000.000        1
 0.45454640E 01 0.26054316E-02-0.10928732E-05 0.20454421E-09-0.14184542E-13    2
-0.54761968E 05 0.18317369E 01 0.34743737E 01 0.16913805E-02 0.73533803E-05    3
-0.99554255E-08 0.36846719E-11-0.54249049E 05 0.83834329E 01                   4
CP                      J 6/62C   1P   100  000  0G   300.000  5000.000        1
 0.37436112E 01 0.53811456E-03-0.34116216E-06 0.63775863E-10-0.44094630E-14    2
 0.54969175E 05 0.42305583E 01 0.32385857E 01 0.51754367E-03 0.35657389E-05    3
-0.48985936E-08 0.18766551E-11 0.55196565E 05 0.72701279E 01                   4
CS                      J12/62C   1S   100  000  0G   300.000  5000.000        1
 0.36942533E 01 0.89086274E-03-0.36600044E-06 0.63778176E-10-0.47810000E-14    2
 0.26452213E 05 0.39176032E 01 0.33093030E 01 0.29164439E-04 0.44317874E-05    3
-0.55253895E-08 0.20392468E-11 0.26658986E 05 0.62942707E 01                   4
CS2                     J 6/61C   1S   20   00   0G   300.000  5000.000        1
 0.59867719E 01 0.16394436E-02-0.68384845E-06 0.12936890E-09-0.89167448E-14    2
 0.12043850E 05-0.63998223E 01 0.32144238E 01 0.10443846E-01-0.11062989E-04    3
 0.52967662E-08-0.83022695E-12 0.12745374E 05 0.76195765E 01                   4
C2                      J 9/61C   200  000  000  0G   300.000  5000.000        1
 0.41718859E 01-0.58280144E-04 0.26982465E-06-0.70416507E-10 0.54949130E-14    2
 0.99055658E 05 0.57669265E 00 0.74313577E 01-0.99823144E-02 0.81154537E-05    3
 0.13955573E-08-0.26415452E-11 0.98305909E 05-0.15764619E 02                   4
C2-                     J 6/66C   2E   100  000  0G   300.000  5000.000        1
 0.36714582E 01 0.80537803E-03-0.30000092E-06 0.52416165E-10-0.34375224E-14    2
 0.62231672E 05 0.31137872E 01 0.47910076E 01-0.21751286E-02 0.80343897E-06    3
 0.24415444E-08-0.16350481E-11 0.61963602E 05-0.25794733E 01                   4
C2F2                    J12/67C   2F   20   00   0G   300.000  5000.000        1
 0.75164581E 01 0.31686462E-02-0.13311365E-05 0.24960049E-09-0.17342072E-13    2
-0.16107655E 03-0.15081225E 02 0.35345837E 01 0.14445845E-01-0.12169692E-04    3
 0.36042985E-08 0.19118951E-12 0.92133562E 03 0.54063023E 01                   4
C2H                     J 3/67C   2H   100  000  0G   300.000  5000.000        1
 0.44207550E 01 0.22119303E-02-0.59294945E-06 0.94195775E-10-0.68527594E-14    2
 0.55835444E 05-0.11582093E 01 0.26499400E 01 0.84913515E-02-0.93165375E-05    3
 0.65373629E-08-0.17356273E-11 0.56275751E 05 0.76898609E 01                   4
C2HF                    J12/67C   2H   1F   10   0G   300.000  5000.000        1
 0.60949501E 01 0.39432429E-02-0.14711438E-05 0.25294641E-09-0.16446663E-13    2
 0.12976907E 05-0.83225076E 01 0.25901770E 01 0.17680853E-01-0.22749855E-04    3
 0.14970568E-07-0.37381925E-11 0.13683223E 05 0.81338073E 01                   4
C2H2                    J 3/61C   2H   200  000  0G   300.000  5000.000        1
 0.45751083E 01 0.51238358E-02-0.17452354E-05 0.28673065E-09-0.17951426E-13    2
 0.25607428E 05-0.35737940E 01 0.14102768E 01 0.19057275E-01-0.24501390E-04    3
 0.16390872E-07-0.41345447E-11 0.26188208E 05 0.11393827E 02                   4
C2H4                    J 9/65C   2H   400  000  0G   300.000  5000.000        1
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 0.34557152E 01 0.11491803E-01-0.43651750E-05 0.76155095E-09-0.50123200E-13    2
 0.44773119E 04 0.26987959E 01 0.14256821E 01 0.11383140E-01 0.79890006E-05    3
-0.16253679E-07 0.67491256E-11 0.53370755E 04 0.14621819E 02                   4
C2N               J 3/67C   2N    100   000   0G    300.000  5000.000          1
 0.61931308E 01 0.14327539E-02-0.61255161E-06 0.11578707E-09-0.80401339E-14    2
 0.64318372E 05-0.84132298E 01 0.32670394E 01 0.98211307E-02-0.83284733E-05    3
 0.17650559E-08 0.59632768E-12 0.65589057E 05 0.65682304E 01                   4
C2N2              J 3/61C   2N    200   000   0G    300.000  5000.000          1
 0.65969935E 01 0.38694131E-02-0.15516161E-05 0.23141546E-09-0.19069442E-13    2
 0.34383726E 05-0.10001801E 02 0.39141782E 01 0.14011008E-01-0.17404350E-04    3
 0.12012779E-07-0.33565772E-11 0.35514550E 05 0.32384353E 01                   4
C2O               J 9/66C   20    100   000   0G    300.000  5000.000          1
 0.48990313E 01 0.28430384E-02-0.10209669E-05 0.16112165E-09-0.95542914E-14    2
 0.32800545E 05-0.91382280E 00 0.35364315E 01 0.69543972E-02-0.53071374E-05    3
 0.17030470E-08-0.14108072E-13 0.33151572E 05 0.60172370E 01                   4
C3               J12/60C   300    000   000   0G    300.000  5000.000          1
 0.47649293E 01 0.27986049E-02-0.11477808E-05 0.21170654E-09-0.14535373E-13    2
 0.93736510E 05-0.28157600E 01 0.28254880E 01 0.80526503E-02-0.62007661E-05    3
 0.20458584E-08-0.11040561E-12 0.94293793E 05 0.72657659E 01                   4
C3O2              J 6/68C   30    20    00    0G    300.000  5000.000          1
 0.81435964E 01 0.54395018E-02-0.22192869E-05 0.40778627E-09-0.27915974E-13    2
-0.14230013E 05-0.15456769E 02 0.37161005E 01 0.19872164E-01-0.20935751E-04    3
 0.11750112E-07-0.26529416E-11-0.13039402E 05 0.69298412E 01                   4
CL                J 3/61CL  100   000   000   0G    300.000  5000.000          1
 0.29595315E 01-0.41899860E-03 0.15980973E-06-0.28102717E-10 0.18673826E-14    2
 0.13659143E 05 0.30350159E 01 0.20888310E 01 0.28675912E-02-0.41905834E-05    3
 0.22408564E-08-0.33258769E-12 0.13836331E 05 0.72655033E 01                   4
CL+               J 6/65CL  1E    -100  000   0G    300.000  5000.000          1
 0.31290605E 01-0.64678626E-03 0.25414315E-06-0.38607442E-10 0.20947135E-14    2
 0.16543856E 06 0.24488638E 01 0.19783295E 01 0.47071709E-02-0.86792897E-05    3
 0.63250309E-08-0.16313361E-11 0.16562590E 06 0.77975420E 01                   4
CL-               J 6/65CL  1E    100   000   0G    300.000  5000.000          1
 0.25000000E 01 0.              0.              0.              0.             2
-0.28874558E 05 0.41872868E 01 0.25000000E 01 0.              0.             3
 0.              0.             -0.28874558E 05 0.41872871E 01                 4
CLCN              J 6/66CL  1C    1N    100   0G    300.000  5000.000          1
 0.54920021E 01 0.20987248E-02-0.77415914E-06 0.13823882E-09-0.92334864E-14    2
 0.14749161E 05-0.37436191E 01 0.33390854E 01 0.10397428E-01-0.13704650E-04    3
 0.95061962E-08-0.25925260E-11 0.15237539E 05 0.68178759E 01                   4
CLF               J 9/65CL  1F    100   000   0G    300.000  5000.000          1
 0.41550345E 01 0.43195995E-03-0.16153995E-06 0.30453169E-10-0.21170113E-14    2
-0.74382198E 04 0.22303893E 01 0.28480871E 01 0.47719011E-02-0.52877698E-05    3
 0.23634468E-08-0.24187423E-12-0.71277966E 04 0.37639116E 01                   4
CLF3              J 9/65CL  1F    300   000   0G    300.000  5000.000          1
 0.89535967E 01 0.11722163E-02-0.50896188E-06 0.97563489E-10-0.68858731E-14    2
-0.22075968E 05-0.18094713E 02 0.28949119E 01 0.24718550E-01-0.35139323E-04    3
 0.22595591E-07-0.53261978E-11-0.20798640E 05 0.11368534E 02                   4
CLO               J 6/61CL  10    100   000   0G    300.000  5000.000          1
 0.40912619E 01 0.50003126E-03-0.18778206E-06 0.35097671E-10-0.24205038E-14    2
 0.10853223E 05 0.36057382E 01 0.28179364E 01 0.44571333E-02-0.44124893E-05    3
 0.15920942E-08-0.14486242E-13 0.11171397E 05 0.10044828E 02                   4
CLO2              J 3/61CL  10    200   000   0G    300.000  5000.000          1
 0.57249758E 01 0.14645230E-02-0.59984351E-06 0.11398750E-09-0.79794776E-14    2
 0.10606264E 05-0.25921838E 01 0.28878166E 01 0.92876003E-02-0.70824040E-05    3
 0.63453376E-09 0.96201605E-12 0.11367377E 05 0.12006873E 02                   4
CL2               J 9/65CL  200   000   000   0G    300.000  5000.000          1
 0.43077814E 01 0.31182816E-03-0.15310807E-06 0.44511913E-10-0.43057753E-14    2
-0.13458251E 04 0.20666664E 01 0.31316986E 01 0.48967877E-02-0.69411463E-05    3
 0.44785641E-08-0.10621859E-11-0.10979696E 04 0.77833424E 01                   4
CL2O             J12/65CL  20    100   000   0G    300.000  5000.000          1
 0.64340062E 01 0.62723309E-03-0.26933252E-06 0.51076394E-10-0.35691545E-14    2
 0.84850530E 04-0.49492767E 01 0.32545238E 01 0.12799449E-01-0.17882460E-04    3
 0.11264333E-07-0.25964252E-11 0.91657423E 04 0.10558058E 02                   4
CS(S)             J 6/63CS  10    00    00    0S    300.000   301.550          1
 0.              0.              0.              0.              0.             2
 0.              0.              0.31827762E 01-0.48703905E-02 0.13369579E-04    3
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 0.89561402E-07-0.24031942E-09-0.96298877E 03-0.75956980E 01                   4
CS(L)               J 6/68CS  10   00   00   0L   301.550  1500.000             1
 0.33149045E 01 0.32287349E-03-0.45641820E-06-0.95936037E-11 0.55471632E-13    2
-0.70109326E 03-0.78759204E 01 0.47696835E 01-0.49137505E-02 0.84861109E-05    3
-0.64184384E-08 0.18034315E-11-0.10158892E 04-0.14960727E 02                   4
CS                  J 6/68CS  10   00   00   0G   300.000  5000.000             1
 0.18710101E 01 0.14068071E-02-0.10636222E-05 0.30523738E-09-0.19977219E-13    2
 0.86814554E 04 0.10235611E 02 0.24999466E 01 0.10332792E-05-0.39771191E-05    3
 0.49283910E-11-0.19810542E-14 0.84737829E 04 0.63527707E 01                   4
CS+                 J 6/68CS  1E  -10   00   0G   300.000  5000.000             1
 0.25000000E 01 0.             0.             0.             0.                2
 0.53653730E 05 0.61694923E 01 0.25000000E 01 0.             0.                3
 0.             0.             0.53653730E 05 0.61694925E 01                   4
CSCL(S)             J 6/68CS  1CL  10   00   0S   300.000   743.000             1
 0.             0.             0.             0.             0.                2
 0.             0.             0.55453400E 01 0.23305834E-02 0.83570330E-06    3
-0.99571640E-09 0.38054803E-12-0.55026535E 05-0.20164260E 02                   4
CSCL(S)             J 6/68CS  1CL  10   00   0S   743.000   918.000             1
 0.             0.             0.             0.             0.                2
 0.             0.             0.81610737E 01-0.17623568E-02-0.22508516E-06    3
 0.39307317E-08-0.23452341E-11-0.55430431E 05-0.33941396E 02                   4
CSCL(L)             J 6/68CS  1CL  10   00   0L   918.000  5000.000             1
 0.93097452E 01 0.             0.             0.             0.                2
-0.55031161E 05-0.40810133E 02 0.93097452E 01 0.             0.                3
 0.             0.            -0.55031161E 05-0.40810133E 02                   4
CSCL                J 6/68CS  1CL  10   00   0G   300.000  5000.000             1
 0.44798455E 01 0.10949164E-03-0.39989914E-08 0.20541995E-12 0.22184640E-16    2
-0.30235809E 05 0.52041565E 01 0.41823030E 01 0.13759553E-02-0.20586233E-05    3
 0.14336474E-08-0.39764546E-12-0.30177927E 05 0.66253273E 01                   4
CSF(S)              J 6/68CS  1F   10   00   0S   300.000   976.000             1
 0.             0.             0.             0.             0.                2
 0.             0.             0.56489993E 01 0.19711398E-02 0.66242382E-06    3
-0.63084871E-09 0.18692339E-12-0.69485102E 05-0.22149959E 02                   4
CSF(L)              J 6/68CS  1F   10   00   0L   976.000  5000.000             1
 0.89071617E 01 0.             0.             0.             0.                2
-0.68066817E 05-0.39912774E 02 0.89071617E 01 0.             0.                3
 0.             0.            -0.68066817E 05-0.39912774E 02                   4
CSF                 J 6/68CS  1F   10   00   0G   300.000  5000.000             1
 0.44373309E 01 0.12715000E-03-0.20547650E-07 0.29813357E-11-0.14774245E-15    2
-0.44227995E 05 0.38803925E 01 0.37449879E 01 0.39100516E-02-0.45883816E-05    3
 0.32179694E-08-0.83786017E-12-0.44090696E 05 0.71317098E 01                   4
CS2                 J 6/68CS  20   00   00   0G   300.000  5000.000             1
 0.46411470E 01 0.10244908E-03 0.10701307E-08 0.55978765E-10-0.77877416E-14    2
 0.11367604E 05 0.76209601E 01 0.45116580E 01 0.17392705E-03 0.36388656E-06    3
-0.41459947E-09 0.16398515E-12 0.11426704E 05 0.83824693E 01                   4
CS2CL2              J 6/68CS  2CL  20   00   0G   300.000  5000.000             1
 0.99424375E 01 0.62659303E-04-0.26331097E-07 0.43912142E-11-0.33554152E-15    2
-0.82345855E 05-0.10611221E 02 0.92952142E 01 0.28505600E-02-0.45576019E-05    3
 0.32557731E-08-0.86067362E-12-0.82222862E 05-0.75315139E 01                   4
CS2F2               J 6/68CS  2F   20   00   0G   300.000  5000.000             1
 0.98793725E 01 0.12674829E-03-0.50905253E-07 0.89711762E-11-0.58090960E-15    2
-0.11005057E 06-0.14067985E 02 0.84425561E 01 0.64921001E-02-0.10832757E-04    3
 0.81791054E-08-0.23173978E-11-0.10978165E 06-0.72614081E 01                   4
E                   L02/67E   10   00   00   0G   300.000  5000.000             1
 0.25000000E 01 0.             0.             0.             0.                2
-0.74537496E 03-0.11734026E 02 0.25000000E 01 0.             0.                3
 0.             0.            -0.74537500E 03-0.11734026E 02                   4
F                   J 9/65F   100  000  000  0G   300.000  5000.000             1
 0.27004353E 01-0.22293182E-03 0.97941385E-07-0.19123038E-10 0.13768154E-14    2
 0.87163617E 04 0.38067182E 01 0.28128740E 01-0.33023098E-05-0.12897310E-05    3
 0.16837365E-08-0.64587833E-12 0.86604019E 04 0.30984198E 01                   4
F-                  J 6/65F   1E   100  000  0G   300.000  5000.000             1
 0.25000000E 01 0.             0.             0.             0.                2
-0.32044752E 05 0.32514845E 01 0.25000000E 01 0.             0.                3
 0.             0.            -0.32044752E 05 0.32514846E 01                   4
FCN                 J 6/61F   1C   1N   100  0G   300.000  5000.000             1
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 0.50921100E 01 0.24183203E-02-0.97912239E-06 0.17890125E-09-0.12194228E-13     2
-0.32576687E 04-0.29666061E 01 0.32675754E 01 0.53659457E-02-0.56599944E-05     3
 0.45438881E-08-0.10902993E-11-0.27875650E 04 0.63587737E 01                    4
FO                  J12/66F   10   100  000  0G   300.000  5000.000             1
 0.39192774E 01 0.70442345E-03-0.26643204E-06 0.49617599E-10-0.33628571E-14     2
 0.11793193E 05 0.33155951E 01 0.29680024E 01 0.26483393E-02-0.37368005E-06     3
-0.19006225E-08 0.10614263E-11 0.12087644E 05 0.83803342E 01                    4
FO2                 J 9/66F   10   200  000  0G   300.000  5000.000             1
 0.57040935E 01 0.13662889E-02-0.58355374E-06 0.10357214E-09-0.75869181E-14     2
-0.39679673E 03-0.20810805E 01 0.37805073E 01 0.61174595E-02-0.55133605E-05     3
 0.17562504E-08 0.67757430E-13 0.12769462E 03 0.78225198E 01                    4
F2                  J12/60F   20   00   00   0G   300.000  5000.000             1
 0.40397806E 01 0.60869035E-03-0.21494672E-06 0.40596803E-10-0.28294433E-14     2
-0.13123536E 04 0.99528039E 00 0.28445997E 01 0.40135072E-02-0.32165655E-05     3
 0.47418780E-09 0.35556237E-12-0.99911761E 03 0.71131622E 01                    4
FE(S)               J 3/65FE  100  000  000  0S   300.000  1184.000             1
 0.40283341E 02-0.25054763E-01-0.24866004E-04 0.11749263E-07 0.47159221E-11     2
-0.20310190E 05-0.23779825E 03 0.32514004E 01-0.72791647E-02 0.34254199E-04     3
-0.49585132E-07 0.26137444E-10-0.83324322E 03-0.14209130E 02                    4
FE(S)               J 3/65FE  100  000  000  0S  1184.000  1665.000             1
 0.32005394E 01 0.75484421E-03 0.             0.             0.                 2
-0.17210443E 03-0.14410926E 02 0.             0.             0.                 3
 0.             0.             0.             0.                                4
FE(S)               J 3/65FE  100  000  000  0S  1665.000  1809.000             1
 0.34018312E 01 0.90581305E-03 0.             0.             0.                 2
-0.59567541E 03-0.16076804E 02 0.             0.             0.                 3
 0.             0.             0.             0.                                4
FE(L)               J 3/65FE  100  000  000  0L  1809.000  5000.000             1
 0.49215842E 01 0.20129179E-03 0.             0.             0.                 2
-0.35541952E 03-0.25191480E 02 0.             0.             0.                 3
 0.             0.             0.             0.                                4
FE                  J 3/65FE  100  000  000  0G   300.000  5000.000             1
 0.34436538E 01-0.14011625E-02 0.81291351E-06-0.16290473E-09 0.12250808E-13     2
 0.49122684E 05 0.25061140E 01 0.25358458E 01 0.37581262E-02-0.99073795E-05     3
 0.90994257E-08-0.28812664E-11 0.49187400E 05 0.59230484E 01                    4
FECL                J 6/65FE  1CL  100  000  0G   300.000  5000.000             1
 0.46940669E 01 0.11604073E-03-0.20840175E-07-0.17626556E-11 0.52313814E-15     2
 0.28730344E 05 0.41803970E 01 0.37885826E 01 0.43678011E-02-0.66922328E-05     3
 0.41797454E-08-0.94686773E-12 0.28920097E 05 0.83402095E 01                    4
FECL2(S)            J 6/65FE  1CL  200  000  0S   300.000   950.000             1
 0.             0.             0.             0.             0.                 2
 0.             0.             0.71307661E 01 0.10951018E-01-0.16731228E-04     3
 0.13155866E-07-0.40011518E-11-0.43600655E 05-0.29072053E 02                    4
FECL2(L)            J 6/65FE  1CL  200  000  0L   950.000  5000.000             1
 0.12288276E 02 0.             0.             0.             0.                 2
-0.41107855E 05-0.53190515E 02 0.12288276E 02 0.             0.                 3
 0.             0.            -0.41107855E 05-0.53190515E 02                    4
FECL2               J 6/65FE  1CL  200  000  0G   300.000  5000.000             1
 0.79569177E 01-0.10430791E-03 0.43393893E-07-0.16106576E-10 0.16163262E-14     2
-0.20226258E 05-0.10752118E 02 0.38434440E 01 0.21564945E-01-0.39937576E-04     3
 0.31321714E-07-0.89050091E-11-0.19671549E 05 0.77677010E 01                    4
FECL3(S)            J 6/65FE  1CL  300  000  0S   300.000   577.000             1
 0.             0.             0.             0.             0.                 2
 0.             0.             0.11306993E 02 0.13230683E-01-0.19156653E-03     3
 0.57778464E-06-0.49463654E-09-0.51600498E 05-0.51237249E 02                    4
FECL3(L)            J 6/65FE  1CL  300  000  0L   577.000  1500.000             1
 0.16102574E 02 0.             0.             0.             0.                 2
-0.48435533E 05-0.67614581E 02 0.16102574E 02 0.             0.                 3
 0.             0.            -0.48435533E 05-0.67614581E 02                    4
FECL3               J 6/65FE  1CL  300  000  0G   300.000  5000.000             1
 0.97771106E 01 0.24421362E-03-0.10313994E-06 0.19207426E-10-0.13179293E-14     2
-0.33439573E 05-0.14562301E 02 0.75614373E 01 0.97332493E-02-0.15543305E-04     3
 0.11126368E-07-0.30022998E-11-0.33013624E 05-0.39929867E 01                    4
FEO(S)              J 6/65FE  1O   100  000  0S   300.000  1650.000             1
 0.58316489E 01 0.14275156E-02-0.93208143E-07-0.65997763E-11-0.22512143E-13     2
-0.34556902E 05-0.26446990E 02 0.53195475E 01 0.22096531E-02 0.10721775E-05     3
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-0.27929729E-08 0.13320733E-11-0.34407165E 05-0.23686034E 02                   4
FEO(L)             J 6/65FE  10   100  000  0L  1650.000  5000.000            1
 0.82022482E 01 0.              0.              0.              0.             2
-0.33345615E 05-0.40079129E 02 0.              0.              0.              3
 0.              0.              0.              0.                            4
FEO                J 9/66FE  10   100  000  0G   300.000  5000.000             1
 0.42049817E 01 0.26834452E-03-0.89426736E-07 0.31855911E-10-0.33922543E-14    2
 0.28829170E 05 0.48172666E 01 0.28245256E 01 0.43049207E-02-0.41984781E-05    3
 0.13201159E-08 0.71316217E-13 0.29194035E 05 0.11578013E 02                   4
FEO2H2             J12/66FE  10   2H   200  0G   300.000  5000.000             1
 0.87960421E 01 0.45844405E-02-0.18808771E-05 0.34177402E-09-0.23047931E-13    2
-0.42754562E 05-0.17856573E 02 0.14918172E 01 0.38499255E-01-0.61500984E-04    3
 0.46635112E-07-0.13308872E-10-0.41450948E 05 0.16384301E 02                   4
FEO2H2(S)          J 6/66FE  10   2H   200  0S   300.000  1500.000             1
 0.74031808E 01 0.11981742E-01-0.14957611E-05-0.50526359E-08 0.20037111E-11    2
-0.71592266E 05-0.34673267E 02 0.10031218E 02 0.44523141E-02 0.40666855E-05    3
-0.40094525E-05 0.23947164E-12-0.72277659E 05-0.48400034E 02                   4
FEO3H3(S)          J 6/66FE  10   3H   300  0S   300.000  1500.000             1
 0.80223926E 01 0.16420135E-01-0.12369378E-06-0.68192838E-08 0.23276907E-11    2
-0.10321336E 06-0.37934020E 02 0.44116836E 01 0.32682462E-01-0.22393815E-04    3
 0.28646792E-08 0.22622321E-11-0.10271834E 06-0.21331014E 02                   4
H                  J 9/65H   100  000  000  0G   300.000  5000.000             1
 0.25000000E 01 0.              0.              0.              0.             2
 0.25471627E 05-0.46011763E 00 0.25000000E 01 0.              0.               3
 0.              0.              0.25471627E 05-0.46011762E 00                 4
H+                 J 6/66H   1E  -100  000  0G   300.000  5000.000             1
 0.25000000E 01 0.              0.              0.              0.             2
 0.18403344E 06-0.11538620E 01 0.25000000E 01 0.              0.               3
 0.              0.              0.18403344E 06-0.11538621E 01                 4
H-                 J 9/65H   1E   100  000  0G   300.000  5000.000             1
 0.25000000E 01 0.              0.              0.              0.             2
 0.15961045E 05-0.11524458E 01 0.25000000E 01 0.              0.               3
 0.              0.              0.15961045E 05-0.11524486E 01                 4
HALO               J 3/64H   1AL  10   100  0G   300.000  5000.000             1
 0.43556053E 01 0.28599933E-02-0.12152821E-05 0.22966419E-09-0.16047592E-13    2
 0.21454053E 04-0.32954978E 01 0.19980220E 01 0.77763784E-02 0.15224672E-05    3
-0.86539734E-08 0.41709380E-11 0.31156301E 04 0.12763795E 02                   4
HBO                J12/64H   1B   1C   100  0G   300.000  5000.000             1
 0.39902765E 01 0.35116761E-02-0.14167746E-05 0.25804765E-09-0.17539792E-13    2
-0.11539403E 05 0.41315742E 00 0.27000640E 01 0.67921406E-02-0.45161135E-05    3
 0.21375092E-08-0.43790703E-12-0.11132099E 05 0.72359559E 01                   4
HBO+               J 6/68H   1B   10   1E  -1G   300.000  5000.000             1
 0.44547347E 01 0.31423614E-02-0.12961293E-05 0.23975605E-09-0.16390748E-13    2
 0.16694872E 06-0.50143149E 00 0.29798548E 01 0.61956382E-02-0.29940031E-05    3
 0.13452306E-09 0.20881907E-12 0.16744444E 06 0.73616124E 01                   4
HBO2               J12/64H   1B   10   200  0G   300.000  5000.000             1
 0.47389519E 01 0.47718771E-02-0.18063494E-05 0.31492889E-09-0.20738312E-13    2
-0.69243338E 05-0.33346713E-02 0.28707366E 01 0.73862644E-02-0.40736842E-06    3
-0.47059022E-08 0.23548893E-11-0.68624111E 05 0.10167820E 02                   4
HCN                J 3/61H   1C   1N   100  0G   300.000  5000.000             1
 0.37415749E 01 0.32984095E-02-0.12102871E-05 0.20523624E-09-0.13190218E-13    2
 0.14395272E 05 0.18847218E 01 0.24471919E 01 0.87763873E-02-0.10219808E-04    3
 0.68998182E-08-0.17913449E-11 0.14653425E 05 0.30959213E 01                   4
HCO                J 3/61H   1C   10   100  0G   300.000  5000.000             1
 0.33366720E 01 0.33912031E-02-0.12957629E-05 0.22679230E-09-0.14952372E-13    2
-0.26430557E 04 0.69479829E 01 0.37929190E 01-0.47861919E-04 0.57306920E-05    3
-0.54606603E-08 0.16[illegible]628E-11-0.26288218E 04 0.52070412E 01           4
HCO+               J 6/66H   1C   10   1E  -1G   300.000  5000.000             1
 0.37043178E 01 0.31689482E-02-0.11162977E-05 0.13295523E-09-0.11423033E-13    2
 0.10159997E 06 0.22646685E 01 0.24008375E 01 0.94708937E-02-0.12325029E-04    3
 [illegible]57365750E-05-0.24046919E-11 0.10131650E 06 0.33016949E 01          4
HCL                J 9/64H   1CL  100  000  0G   300.000  5000.000             1
 0.27665954E 01 0.14381883E-02-0.46993000E-06 0.73499408E-10-0.43731106E-14    2
-0.11917468E 05 0.64583540E 01 0.35248171E 01 0.29924862E-04-0.86221891E-06    3
 0.20979721E-08-0.98658191E-12-0.12150509E 05 0.23957713E 01                   4
HF                 J12/63H   1F   100  000  0G   300.000  5000.000             1
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 0.30075250E 01 0.68441682E-03-0.49447506E-07-0.16420127E-10 0.23547944E-14   2
-0.33454373E 05 0.37266479E 01 0.34614364E 01 0.35564235E-03-0.10911244E-05   3
 0.12931449E-08-0.40567002E-12-0.33648707E 05 0.10945702E 01                 4
H02                J 3/64H   10   200  000  0G   300.000  5000.000           1
 0.37866280E 01 0.27885404E-02-0.10169708E-05 0.17193946E-09-0.11021852E-13   2
 0.11888500E 04 0.48147611E 01 0.35094850E 01 0.11496670E-02 0.58784259E-05   3
-0.77735519E-08 0.29607883E-11 0.13803331E 04 0.68276325E 01                 4
H2                 J 3/61H   20   00   00   0G   300.000  5000.000            1
 0.31001901E 01 0.51119464E-03 0.52644210E-07-0.34909973E-10 0.36945345E-14   2
-0.87738042E 03-0.19629421E 01 0.30574451E 01 0.26765200E-02-0.58099162E-05   3
 0.55210391E-08-0.18122739E-11-0.98890474E 03-0.22997056E 01                 4
H2O(S)             L11/65H   20   100  000  0S   200.000   273.150            1
 0.             0.             0.             0.             0.               2
 0.             0.            -0.39269330E-01 0.16920420E-01 0.               3
 0.             0.            -0.35949581E 05 0.55933784E 00                 4
H2O(L)             L11/65H   20   100  000  0L   273.150   373.150            1
 0.             0.             0.             0.             0.               2
 0.             0.             0.12712782E 02-0.17662790E-01-0.22556661E-04   3
 0.20820908E-06-0.24078614E-09-0.37483200E 05-0.59115345E 02                 4
H2O                J 3/61H   20   100  000  0G   300.000  5000.000            1
 0.27167633E 01 0.29451374E-02-0.80224374E-06 0.10226682E-09-0.48472145E-14   2
-0.29905826E 05 0.66305671E 01 0.40701275E 01-0.11084499E-02 0.41521180E-05   3
-0.29637404E-08 0.80702103E-12-0.30279722E 05-0.32270046E 00                 4
H2S                J12/65H   2S   100  000  0G   300.000  5000.000            1
 0.28479103E 01 0.38415990E-02-0.14099367E-05 0.24278754E-09-0.15783283E-13   2
-0.34469738E 04 0.74791412E 01 0.35811293E 01-0.13211856E-03 0.36517726E-05   3
-0.21820445E-08 0.28723779E-12-0.36350917E 04 0.25161511E 01                 4
H3B306             J12/64H   3B   30   600  0G   300.000  5000.000            1
 0.20153579E 02 0.13016286E-01-0.59669619E-05 0.90308253E-09-0.60532410E-13   2
-0.28104092E 06-0.79689531E 02-0.22705116E 01 0.87024894E-01-0.91587714E-04   3
 0.39445392E-07-0.36666035E-11-0.27569523E 06 0.32516454E 02                 4
HE                 L 5/66HE  100  000  000  0G   300.000  5000.000            1
 0.25000000E 01 0.             0.             0.             0.               2
-0.74537493E 03 0.91534888E 00 0.25000000E 01 0.             0.               3
 0.             0.            -0.74537498E 03 0.91534884E 00                 4
HE+                L12/66HE  1E   -100  000  0G   300.000  5000.000           1
 0.25000000E 01 0.             0.             0.             0.               2
 0.28534266E 06 0.16084045E 01 0.25000000E 01 0.             0.               3
 0.             0.             0.28534266E 06 0.16084046E 01                 4
K(S)               J12/61K   10   00   00   0S   300.000   336.350            1
 0.             0.             0.             0.             0.               2
 0.             0.             0.17263229E 01-0.98042772E-04 0.13852978E-04   3
 0.57915802E-07-0.11734935E-09-0.69166994E 03-0.23234372E 01                 4
K(L)               J12/61K   10   00   00   0L   336.350  2000.000            1
 0.32625048E 01-0.13113792E-03 0.50811991E-06 0.62810507E-10-0.51130459E-13   2
-0.52525237E 03-0.36002325E 01 0.44202110E 01-0.19475966E-02 0.61695016E-06   3
 0.59316043E-09-0.33655604E-12-0.96275784E 03-0.16042433E 02                 4
K                  J 6/62K   100  000  000  0G   300.000  5000.000            1
 0.25673650E 01-0.14933596E-03 0.12342444E-06-0.53394240E-10 0.11948426E-13   2
 0.99559531E 04 0.46642081E 01 0.24930967E 01 0.50164177E-04-0.12751224E-06   3
 0.13540491E-09-0.51145936E-13 0.99786360E 04 0.50560438E 01                 4
K+                 J 3/65K   1E   -100  000  0G   300.000  5000.000           1
 0.25000000E 01 0.             0.             0.             0.               2
 0.61096558E 05 0.43339455E 01 0.25000000E 01 0.             0.               3
 0.             0.             0.61096558E 05 0.43339455E 01                 4
KCL(S)             J 3/66K   1CL  100  000  0S   300.000  1044.000            1
 0.89157169E 01-0.20927271E-02 0.47310182E-05 0.70152537E-09-0.55146099E-11   2
-0.52747066E 05-0.10144700E 02 0.53934311E 01 0.26535242E-02 0.96075655E-06   3
-0.50251843E-08 0.40721228E-11-0.54748389E 05-0.21536814E 02                 4
KCL(L)             J 3/66K   1CL  100  000  0L  1044.000  5000.000            1
 0.88518064E 01 0.             0.             0.             0.               2
-0.53369478E 05-0.40010059E 02 0.             0.             0.               3
 0.             0.             0.             0.                             4
KCL                J 3/66K   1CL  100  000  0G   300.000  5000.000            1
 0.44636733E 01 0.12229207E-03-0.91719210E-08 0.92645242E-12-0.10407917E-16   2
-0.27173133E 05 0.32349330E 01 0.39908569E 01 0.21089169E-02-0.31836530E-05   3
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 0.22525308E-08-0.59094179E-12-0.27080184E 05 0.54988475E 01                   4
KO                  J12/62K   10    100  000  0S    300.000  5000.000          1
 0.43731489E 01 0.19960449E-03-0.56826345E-07 0.10410356E-10-0.70291368E-15    2
 0.37491801E 04 0.32551045E 01 0.33905135E 01 0.41932012E-02-0.61235594E-05    3
 0.40675370E-08-0.99172754E-12 0.39512947E 04 0.80473015E 01                   4
K2                  J12/61K   200   000  000  0G    300.000  5000.000          1
 0.45039995E 01 0.22596406E-03 0.14957172E-07-0.34811532E-11 0.34052376E-15    2
 0.13926067E 05 0.42568563E 01 0.44424903E 01 0.46158726E-03-0.30025595E-06    3
 0.17502910E-09-0.32470554E-13 0.13941670E 05 0.45868357E 01                   4
K2O(S)              J 6/63K   20    100  000  0S    300.000  2000.000          1
 0.86890737E 01 0.51097498E-02-0.20386508E-06 0.58747271E-10-0.10899823E-14    2
-0.46449235E 05-0.39589233E 02 0.34449681E 01 0.40567031E-01-0.52051685E-04    3
 0.79006086E-07-0.27313775E-10-0.45925458E 05-0.17385210E 02                   4
LI(S)               J 6/62LI  10    00   00   0S    300.000   453.690          1
 0.             0.             0.             0.             0.                2
 0.             0.             0.91818617E 01-0.35999310E-01 0.24881854E-05    3
 0.26456527E-06-0.34331039E-09-0.15159533E 04-0.39545554E 02                   4
LI(L)               J 6/62LI  10    00   00   0L    453.690  4000.000          1
 0.36114162E 01-0.18325283E-03 0.40743757E-07 0.26515630E-11-0.11572503E-14    2
-0.74925732E 03-0.16352732E 02 0.35988094E 01 0.61335444E-03-0.48307646E-05    3
 0.61290368E-08-0.23400340E-11-0.87493582E 03-0.18156235E 02                   4
LI                  J 6/62LI  100   000  000  0G    300.000  5000.000          1
 0.24737658E 01 0.87435341E-04-0.93773573E-07 0.31327924E-10-0.17579908E-14    2
 0.18568036E 05 0.25630288E 01 0.25103738E 01-0.74235738E-04 0.18612567E-06    3
-0.19540947E-09 0.73145266E-13 0.18581670E 05 0.23902453E 01                   4
LI+                 J 3/65LI  1E   -100  000  0G    300.000  5000.000          1
 0.25000900E 01 0.             0.             0.             0.                2
 0.81899068E 05 0.17406170E 01 0.25000000E 01 0.             0.                3
 0.             0.             0.81899068E 05 0.17406170E 01                   4
LICL(S)             J 6/62LI  1CL   100  000  0S    300.000   883.000          1
 0.             0.             0.             0.             0.                2
 0.             0.             0.41095245E 01 0.81381003E-02-0.11541874E-04    3
 0.10553538E-07-0.36457022E-11-0.50608268E 05-0.13298894E 02                   4
LICL(L)             J 6/62LI  1CL   100  000  0L    883.000  2000.000          1
 0.82149477E 01 0.56391361E-03-0.17359331E-05 0.76595005E-09-0.12378477E-12    2
-0.50007322E 05-0.33808961E 02 0.10383028E 02-0.47179659E-02-0.16138317E-05    3
 0.80807174E-08-0.44459493E-11-0.50539120E 05-0.49921960E 02                   4
LICL                J 6/62LI  1CL   100  000  0G    300.000  5000.000          1
 0.42712143E 01 0.31400791E-03-0.10123[illegible]E-06 0.18451853E-10-0.12398731E-14    2
-0.24884442E 05 0.10285692E 01 0.29906905E 01 0.53338642E-02-0.65671979E-05    3
 0.38050160E-08-0.76117455E-12-0.24603182E 05 0.73150321E 01                   4
LIF(S)              J12/63LI  1F    100  000  0S    300.000  1121.300          1
 0.57937896E 01-0.49996725E-03 0.16287053E-05 0.12938534E-08-0.10559079E-11    2
-0.75511641E 05-0.28854332E 02 0.17624503E 01 0.17550874E-01-0.28143548E-04    3
 0.22393192E-07-0.68974890E-11-0.74816904E 05-0.93175903E 01                   4
LIF(L)              J12/63LI  1F    100  000  0L   1121.300  5000.000          1
 0.77191711E 01 0.             0.             0.             0.                2
-0.73822749E 05-0.38813129E 02 0.             0.             0.                3
 0.             0.             0.             0.                               4
LIF                 J12/63LI  1F    100  000  0G    300.000  5000.000          1
 0.40476615E 01 0.56143535E-03-0.20377763E-06 0.39160917E-10-0.27107864E-14    2
-0.41317801E 05 0.65825575E 00 0.28628366E 01 0.38823430E-02-0.29952641E-05    3
 0.24730751E-09 0.43954489E-12-0.41005091E 05 0.67357165E 01                   4
LIFO                J 9/65LI  1F    10   100  0G    300.000  5000.000          1
 0.59926109E 01 0.11139200E-02-0.47888493E-06 0.91068332E-10-0.63849123E-14    2
-0.13100989E 05-0.53497665E 01 0.25001790E 01 0.12661717E-01-0.14157559E-04    3
 0.64506374E-08-0.74261431E-12-0.12265534E 05 0.12130855E 02                   4
LIH(S)              J 9/67LI  1H    100  000  0S    300.000   961.800          1
 0.             0.             0.             0.             0.                2
 0.             0.             0.75118128E 00 0.12127957E-01-0.86900336E-05    3
 0.56311555E-08-0.12693483E-11-0.11486991E 05-0.39654575E 01                   4
LIH(L)              J 9/67LI  1H    100  000  0L    961.800  5000.000          1
 0.74981191E 01 0.             0.             0.             0.                2
-0.11581326E 05-0.40047273E 02 0.74981191E 01 0.             0.                3
 0.             0.            -0.11581826E 05-0.40047278E 02                   4
LIH                 J 9/67LI  1H    100  000  0G    300.000  5000.000          1
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 0.35884297E 01 0.10727691E-02-0.40194588E-06 0.73828557E-10-0.49269644E-14    2
 0.15717625E 05-0.38820950F 00 0.34209486F 01-0.69067366E-03-0.56527381E-05    3
-0.62180348E-08 0.21531755E-11 0.15834945E 05 0.10525714E 01                   4
LIN             J12/66LI  1N   100  000  0G   300.000  5000.000                1
 0.42258077E 01 0.39667187E-03-0.12493993E-06 0.23174759E-10-0.15851917E-14    2
 0.33916952E 05 0.63765563E 00 0.28894300E 01 0.52212534E-02-0.65759021F-05    3
 0.37288997E-08-0.72355143E-12 0.39216323E 05 0.72757056E 01                   4
LIO             J 3/64LI  10   100  000  0G   300.000  5000.000                1
 0.41876205E 01 0.41186574E-03-0.14520296E-06 0.27253070E-10-0.18864775E-14    2
 0.87795259E 04 0.12182630E 01 0.28389007F 01 0.51538626E-02-0.63082382E-05    3
 0.34114385E-08-0.61631343E-12 0.90334314E 04 0.73959549F 01                   4
LIO-            J12/67LI  10   1E   10   0G   300.000  5000.000                1
 0.41810217E 01 0.41785000F-03-0.15024845E-06 0.28397732E-10-0.19789181E-14    2
-0.93549702E 04-0.15555110E 00 0.28515866E 01 0.59169880E-02-0.59547475E-05    3
 0.30399451E-08-0.47872969E-12-0.90778076E 04 0.64462719F 01                   4
LIOH(S)         J 3/66LI  10   1H   100  0S   300.000   744.300                1
 0.             0.             0.             0.             0.                2
 0.             0.             0.63640356E-01 0.30407660E-01-0.44034005E-04    3
 0.30692106E-07-0.66439718E-11-0.59331340E 05-0.25794094E 01                   4
LIOH(L)         J 3/66LI  10   1H   100  0L   744.300  5000.000                1
 0.10436979E 02 0.             0.             0.             0.                2
-0.60109250E 05-0.53641166E 02 0.10436979E 02 0.             0.                3
 0.             0.            -0.60109250E 05-0.53641166E 02                   4
LIOH            J 3/66LI  10   1H   100  0G   300.000  5000.000                1
 0.40456064E 01 0.23824852E-02-0.82302724E-06 0.13279161E-09-0.81929541E-14    2
-0.31003210E 05 0.22550447E 01 0.32569330E 01 0.30440910E-02 0.25371683E-05    3
-0.55730639E-08 0.24765340E-11-0.30730637E 05 0.66566487F 01                   4
LICN            J 9/66LI  10   1N   100  0G   300.000  5000.000                1
 0.58123496E 01 0.12870625E-02-0.54667710E-06 0.10314987E-09-0.71930447F-14    2
 0.19692302E 05-0.43578702E 01 0.36701164E 01 0.72568177E-02-0.58681146E-05    3
 0.11628312E-08 0.42704122E-12 0.20271703E 05 0.66633305E 01                   4
LI2             J 6/62LI  200  000  000  0S   300.000  5000.000                1
 0.44338756E 01 0.22848941E-03-0.24519024E-07 0.39448820E-11-0.22839492E-15    2
 0.24005747E 05-0.17116905E 01 0.37418914E 01 0.31246294E-02-0.46337063E-05    3
 0.32618304E-08-0.85308216E-12 0.24142156E 05 0.16040721E 01                   4
LI2CL2          J 6/62LI  2CL  200  000  0G   300.000  5000.000                1
 0.95245614E 01 0.52458834E-03-0.22337949F-06 0.41951114E-10-0.29021306E-14    2
-0.74990263E 05-0.20044824E 02 0.52801351E 01 0.13384100E-01-0.28759448E-04    3
 0.28313359E-07-0.53433247E-11-0.74160003E 05 0.26612705E 00                   4
LI2F2           J12/63LI  2F   200  000  0G   300.000  5000.000                1
 0.92241415E 01 0.87023522E-03-0.37828706E-06 0.72506822E-10-0.51157843E-14    2
-0.11450290E 06-0.21319163E 02 0.35813313E 01 0.23905498E-01-0.36100653E-04    3
 0.24668598E-07-0.62706615E-11-0.11336586E 06 0.53542154E 01                   4
LI2O(S)         J 3/64LI  20   100  000  0S   300.000  1843.000                1
 0.42774776E 01 0.73521672E-02-0.52225090E-06-0.17364426E-08 0.53961035E-12    2
-0.73396278E 05-0.21765497E 02-0.31727239E 00 0.36149356E-01-0.55455921E-04    3
 0.41796437E-07-0.11804048E-10-0.73106196E 05-0.22888330E 01                   4
LI2O(L)         J 3/64LI  20   100  000  0L  1843.000  5000.000                1
 0.12076931E 02 0.             0.             0.             0.                2
-0.71337921E 05-0.65174974E 02 0.             0.             0.                3
 0.             0.             0.             0.                               4
LI2O            J 3/64LI  20   100  000  0G   300.000  5000.000                1
 0.65193748E 01 0.96879443E-03-0.41490506E-06 0.78637337E-10-0.54969292E-14    2
-0.22255325E 05-0.10834722E 02 0.39721708E 01 0.97460921E-02-0.93596149E-05    3
 0.34639160E-08-0.75658880F-13-0.21596988E 05 0.25391411E 01                   4
LI2O2           J 3/64LI  20   200  000  0G   300.000  5000.000                1
 0.95275260E 01 0.53021013E-03-0.23005862E-06 0.44030831E-10-0.31018702E-14    2
-0.32132434E 05-0.21872279E 02 0.55375232E 01 0.17344223E-01-0.27197971E-04    3
 0.19395629E-07-0.51207957E-11-0.31407044F 05-0.27814759E 01                   4
LI2O2H2         J 3/66LI  2O   2H   200  0G   300.000  5000.000                1
 0.89420600E 01 0.60583335F-02-0.22032892E-05 0.37293081E-09-0.24009566F-13    2
-0.94593042E 05-0.21057433E 02 0.28083766E 01 0.24969790E-01-0.21603225E-04    3
 0.63288723E-08 0.64221372E-12-0.93070570E 05 0.99492004E 01                   4
LI3CL3          J 6/62LI  3CL  300  000  0G   300.000  5000.000                1
 0.14319440E 02 0.18854007E-02-0.81378330E-06 0.15735494E-09-0.11119472E-13    2
-0.12553351E 06-0.42724179E 02 0.45745959E 01 0.39749239E-01-0.56508213E-04    3
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 0.36294145E-07-0.85784700E-11-0.12353351E 06 0.45674442E 01                 4
LI3F3              J12/63LI  3F   300  000  0G   300.000  5000.000           1
 0.13091417E 02 0.32374694E-02-0.14000897E-05 0.25766663E-09-0.18855216E-13  2
-0.18679660E 06-0.41168173E 02 0.14982352E 01 0.43683009E-01-0.53290482E-04  3
 0.23105860E-07-0.45220108E-11-0.13412906E 06 0.16334742E 02                 4
MG(S)              J 9/62MG  10   00   00   0S   300.000   922.000           1
 0.             0.             0.             0.             0.              2
 0.             0.             0.20184771E 01 0.52525745E-02-0.89160059E-05  3
 0.81194529E-08-0.23538706E-11-0.77246715E 03-0.88131212E 01                 4
MG(L)              J 9/62MG  10   00   00   0L   922.000  5000.000           1
 0.26570516E 01 0.13083966E-02 0.             0.             0.              2
 0.22868300E 03-0.10433817E 02 0.26570516E 01 0.13083966E-02 0.              3
 0.             0.             0.22868300E 03-0.10433817E 02                 4
MG                 J 9/62MG  100  000  000  0G   300.000  5000.000           1
 0.24188605E 01 0.16145771E-03-0.99399205E-07 0.18989312E-10 0.91656165E-16  2
 0.17036992E 05 0.40641123E 01 0.24988751E 01 0.87608205E-05-0.23614632E-07  3
 0.26287528E-10-0.10308811E-13 0.17008321E 05 0.36263633E 01                 4
MG+                J12/67MG  1E   -10  00   0G   300.000  5000.000           1
 0.25084828E 01-0.17499680E-04 0.12102317E-07-0.34320303E-11 0.34653473E-15  2
 0.10571437E 06 0.42685235E 01 0.24961675E 01 0.27410788E-04-0.68663780E-07  3
 0.72015616E-10-0.26930064E-13 0.10571774E 06 0.43307379E 01                 4
MGCL               J 3/66MG  1CL  100  000  0G   300.000  5000.000           1
 0.43775833E 01 0.18834173E-03-0.54435592E-07 0.99491031E-11-0.66949611E-15  2
-0.65830826E 04 0.29762332E 01 0.33800534E 01 0.42813389E-02-0.64457333E-05  3
 0.44472291E-08-0.11421727E-11-0.63826560E 04 0.77758327E 01                 4
MGCL+              J 6/68MG  1CL  1E   -10  0G   300.000  5000.000           1
 0.63512344E 01-0.37967190E-02 0.24712945E-05-0.50823653E-09 0.33672625E-13  2
 0.76480879E 05-0.83035040E 01 0.36012230E 01 0.34791859E-02-0.51353143E-05  3
 0.34446337E-08-0.83848206E-12 0.77314688E 05 0.61207176E 01                 4
MGCLF              J 3/66MG  1CL  1F   100  0G   300.000  5000.000           1
 0.55536109E 01 0.49503794E-03-0.21265567E-06 0.40342907E-10-0.28198241E-14  2
-0.70522498E 05-0.61610398E 01 0.39675363E 01 0.10495156E-01-0.14846158E-04  3
 0.94797313E-08-0.22227485E-11-0.69974510E 05 0.64280836E 01                 4
MGCL2(S)           J12/65MG  1CL  200  000  0S   300.000   987.000           1
 0.             0.             0.             0.             0.              2
 0.             0.             0.54491296E 01 0.16745224E-01-0.25956907E-04  3
 0.19111573E-07-0.51059014E-11-0.79343894E 05-0.24261034E 02                 4
MGCL2(L)           J12/65MG  1CL  200  000  0L   987.000  5000.000           1
 0.11071048E 02 0.             0.             0.             0.              2
-0.76294618E 05-0.48972588E 02 0.11071048E 02 0.             0.              3
 0.             0.            -0.76294618E 05-0.48972588E 02                 4
MGCL2              J12/65MG  1CL  200  000  0G   300.000  5000.000           1
 0.66909609E 01 0.34055850E-03-0.14507415E-06 0.27277270E-10-0.18898997E-14  2
-0.50324903E 05-0.57763697E 01 0.44799697E 01 0.92698674E-02-0.13850184E-04  3
 0.93638025E-08-0.23516224E-11-0.49874382E 05 0.48946211E 01                 4
MGF                J 3/67MG  1F   100  000  0G   300.000  5000.000           1
 0.42110735E 01 0.36113259E-03-0.13239533E-06 0.24644432E-10-0.16919094E-14  2
-0.28059832E 05 0.23145832E 01 0.28664199E 01 0.51658813E-02-0.65086664E-05  3
 0.36302039E-08-0.69177563E-12-0.27754352E 05 0.39564751E 01                 4
MGF2(S)            J 3/66MG  1F   200  000  0S   300.000  1536.000           1
 0.66953750E 01 0.43929183E-02-0.11903584E-05-0.53362104E-09 0.31219775E-12  2
-0.13736474E 06-0.32490950E 02 0.21304889E 01 0.28542721E-01-0.45495513E-04  3
 0.33548644E-07-0.91548251E-11-0.13678478E 06-0.12050724E 02                 4
MGF2(L)            J 3/66MG  1F   200  000  0L  1536.000  5000.000           1
 0.11357899E 02 0.             0.             0.             0.              2
-0.13400296E 06-0.57018423E 02 0.             0.             0.              3
 0.             0.             0.             0.                            4
MGF2               J 3/66MG  1F   200  000  0G   300.000  5000.000           1
 0.64284568E 01 0.63969935E-03-0.27809763E-06 0.53430244E-10-0.37812854E-14  2
-0.89226616E 05-0.60380744E 01 0.37706721E 01 0.10406351E-01-0.13695278E-04  3
 0.80146506E-08-0.16568864E-11-0.88639643E 05 0.70214053E 01                 4
MGH                J12/66MG  1H   100  000  0G   300.000  5000.000           1
 0.34638591E 01 0.12404055E-02-0.50278210E-06 0.93118834E-10-0.66183068E-14  2
 0.13176310E 05 0.29845865E 01 0.35102397E 01-0.12368352E-02 0.64246998E-05  3
-0.65054346E-08 0.22003625E-11 0.19293893E 05 0.33504888E 01                 4
MGN                J 3/64MG  1N   100  000  0G   300.000  5000.000           1
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 0.42214417E 01 0.36489240E-03-0.12995730E-06 0.24419940E-10-0.16917759E-14    2
 0.33392931E 05 0.27188874E 01 0.28894549E 01 0.51757175E-02-0.65849016E-05    3
 0.37218933E-08-0.72385964E-12 0.33681058E 05 0.92844249E 01                   4
MGO(S)              J12/65MG  10   100  000  0S   300.000  3098.000            1
 0.51120198E 01 0.17231664E-02-0.90268818E-06 0.26460605E-09-0.28339967E-13    2
-0.74084363E 05-0.26784367E 02 0.47740339E 00 0.21441338E-01-0.33453071E-04    3
 0.24347437E-07-0.66578961E-11-0.73154228E 05-0.45934874E 01                   4
MGO(L)              J12/65MG  10   100  000  0L  3098.000  5000.000            1
 0.72964786E 01 0.             0.             0.             0.                2
-0.67744028E 05-0.38362761E 02 0.             0.             0.                3
 0.             0.             0.             0.                               4
MGO                 J12/65MG  10   100  000  0G   300.000  5000.000            1
 0.40654306E 01 0.54784296E-03-0.19704758E-06 0.36606637E-10-0.25102520E-14    2
-0.81403801E 03 0.31030930E 01 0.28442075E 01 0.41055545E-02-0.35061249E-05    3
 0.72885498E-09 0.27783028E-12-0.49777511E 03 0.93349957E 01                   4
MGOH                J 6/67MG  10   1H   100  0G   300.000  5000.000            1
 0.44328606E 01 0.25811369E-02-0.91887753E-06 0.15151434E-09-0.93758909E-14    2
-0.27755885E 05 0.25918925E 00 0.16842602E 01 0.10914848E-01-0.87026993E-05    3
 0.13336126E-08 0.94723703E-12-0.27081380E 05 0.14150863E 02                   4
MGOH+               J 6/66MG  10   1H   1E  -10   300.000  5000.000            1
 0.47424330E 01 0.22877007E-02-0.80398933E-06 0.13175298E-09-0.82324460E-14    2
 0.70323806E 05-0.18812567E 01 0.17246936E 01 0.13231006E-01-0.14929146E-04    3
 0.73413788E-08-0.10182671E-11 0.70977879E 05 0.12933122E 02                   4
MGO2H2              J 6/67MG  10   2H   200  0G   300.000  5000.000            1
 0.73269210E 01 0.49370374E-02-0.18021108E-05 0.30460208E-09-0.19535992E-13    2
-0.71137802E 05-0.10591697E 02 0.42789288E 01 0.15680923E-01-0.15568577E-04    3
 0.74423876E-08-0.10867487E-11-0.70438934E 05 0.44897963E 01                   4
N                   J 3/61N  100   000  000  0G   300.000  5000.000            1
 0.24502682E 01 0.10661458E-03-0.74653373E-07 0.18796524E-10-0.10259839E-14    2
 0.56116040E 05 0.44487581E 01 0.25030714E 01-0.21800181E-04 0.54205287E-07    3
-0.56475602E-10 0.20999044E-13 0.56098904E 05 0.41675764E 01                   4
NF                  J 6/65N   1F   100  000  0G   300.000  5000.000            1
 0.38624046E 01 0.74409961E-03-0.29304178E-06 0.55130022E-10-0.38317928E-14    2
 0.28669390E 05 0.34570237E 01 0.30480680E 01 0.19566867E-02 0.94322448E-06    3
-0.29336643E-08 0.13504454E-11 0.28941633E 05 0.79992363E 01                   4
NF2                 J 3/64N   1F   200  000  0G   300.000  5000.000            1
 0.57186890E 01 0.14102822E-02-0.60493363E-06 0.11491911E-09-0.80536431E-14    2
 0.30992968E 04-0.34469259E 01 0.25009872E 01 0.10721062E-01-0.92064150E-05    3
 0.19027666E-08 0.71249647E-12 0.39376954E 04 0.12994042E 02                   4
NF3                 J 3/64N   1F   300  000  0G   300.000  5000.000            1
 0.79754975E 01 0.22473716E-02-0.97077542E-06 0.18551042E-09-0.13066945E-13    2
-0.18151986E 05-0.15632481E 02 0.12579876E 01 0.24357895E-01-0.27038511E-04    3
 0.12176078E-07-0.13589121E-11-0.16539966E 05 0.13018394E 02                   4
NH                  J12/65N   1H   100  000  0G   300.000  5000.000            1
 0.27741580E 01 0.13179393E-02-0.38379707E-06 0.54142146E-10-0.28838332E-14    2
 0.39959049E 05 0.57923234E 01 0.34889532E 01 0.28026519E-03-0.13456768E-05    3
 0.22939931E-08-0.95757540E-12 0.39714793E 05 0.18654962E 01                   4
NH2                 J12/65N   1H   200  000  0G   300.000  5000.000            1
 0.25769524E 01 0.35896090E-02-0.12276328E-05 0.19549576E-09-0.11873401E-13    2
 0.19335912E 05 0.79074890E 01 0.40385791E 01-0.10098163E-02 0.40120903E-05    3
-0.23085312E-08 0.39022337E-12 0.18973010E 05 0.52464285E 00                   4
NH3                 J 9/65N   1H   300  000  0G   300.000  5000.000            1
 0.24165177E 01 0.61871211E-02-0.21785136E-05 0.37599009E-09-0.24448856E-13    2
-0.64747177E 04 0.77043482E 01 0.35912768E 01 0.49388668E-03 0.83449322E-05    3
-0.83833385E-08 0.27299092E-11-0.66717143E 04 0.22520966E 01                   4
NO                  J 6/63N   10   100  000  0G   300.000  5000.000            1
 0.31890000E 01 0.13382281E-02-0.52899318E-06 0.95919332E-10-0.64847932E-14    2
 0.98283290E 04 0.67458126E 01 0.40459521E 01-0.34181783E-02 0.79819190E-05    3
-0.61139316E-08 0.15919076E-11 0.97453934E 04 0.29974988E 01                   4
NO+                 J 6/66N   10   1E  -100  0G   300.000  5000.000            1
 0.28885488E 01 0.15217119E-02-0.57531241E-06 0.10051031E-09-0.66044294E-14    2
 0.11819245E 06 0.70027197E 01 0.36685056E 01-0.11544520E-02 0.21755608E-05    3
-0.48227472E-09-0.27847906E-12 0.11803369E 06 0.31779324E 01                   4
NOCL                J12/65N   10   1CL  100  0G   300.000  5000.000            1
 0.54195728E 01 0.18136694E-02-0.66876691E-06 0.12297226E-09-0.84070919E-14    2
 0.44171536E 04-0.19183566E 00 0.49280308E 01 0.59426529E-02-0.55620366E-05    3
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 0.29353736E-08-0.66517496E-12 0.44034480E 04 0.69547732E 01                   4
NOF                 J 6/61N   10    1F    100   0G    300.000  5000.000        1
 0.51906668E 01 0.13924266E-02-0.79642361E-06 0.14626364E-09-0.10097419E-13    2
-0.96758164E 04-0.62298477E 00 0.32902070E 01 0.74045493E-02-0.66195803E-05    3
 0.26529282E-08-0.29526815E-12-0.91566645E 04 0.31451185E 01                   4
NO2                 J 9/64N   10    200   000   0G    300.000  5000.000        1
 0.46240771E 01 0.25260332E-02-0.10609499E-05 0.19879239E-09-0.13799384E-13    2
 0.22899900E 04 0.13324138E 01 0.34589236E 01 0.20647064E-02 0.66966067E-05    3
-0.95556725E-08 0.36195881E-11 0.28152265E 04 0.83116983E 01                   4
NO2-                J12/65N   10    2E    100   0G    300.000  5000.000        1
 0.50794422E 01 0.20860322E-02-0.89523762E-06 0.16901079E-09-0.11743414E-13    2
-0.45039907E 05-0.16367650E 01 0.29474526E 01 0.51836832E-02 0.24205126E-05    3
-0.75758344E-08 0.34577493E-11-0.44317583E 05 0.10052399E 02                   4
NO2CL               J12/65N   10    2CL   100   0G    300.000  5000.000        1
 0.72062138E 01 0.29949809E-02-0.12641260E-05 0.23758750E-09-0.16524848E-13    2
-0.11366123E 04-0.99256667E 01 0.35302225E 01 0.14573930E-01-0.11645930E-04    3
 0.25890139E-08 0.64589481E-12 0.76652034E 01 0.11618599E 02                   4
NO2F                J12/65N   10    2F    100   0G    300.000  5000.000        1
 0.69639166E 01 0.33554437E-02-0.14158297E-05 0.26622227E-09-0.18531606E-13    2
-0.15621287E 05-0.95806218E 01 0.22424380E 01 0.162[illegible]-01-0.13344332E-04    3
 0.32719525E-08 0.59144703E-12-0.14364205E 05 0.14218996E 02                   4
N2                  J 9/65N   20    00    00    0G    300.000  5000.000        1
 0.28963194E 01 0.15154866E-02-0.57235277E-06 0.99807393E-10-0.65223555E-14    2
-0.90586184E 03 0.61615148E 01 0.36748261E 01-0.12081500E-02 0.23240102E-05    3
-0.63217559E-09-0.22577253E-12-0.10611588E 04 0.23580424E 01                   4
N2C                 J 6/66N   2C    100   000   0G    300.000  5000.000        1
 0.59145719E 01 0.17176878E-02-0.73057492E-06 0.13812907E-09-0.96540216E-14    2
 0.49688947E 05-0.73960996E 01 0.28823173E 01 0.10961803E-01-0.10399571E-04    3
 0.38588460E-08-0.17324120E-12 0.50474679E 05 0.30410089E 01                   4
N2H4                J12/65N   2H    400   000   0G    300.000  5000.000        1
 0.50947770E 01 0.93296138E-02-0.33626986E-05 0.56308304E-09-0.35859661E-13    2
 0.92996644E 04-0.35950952E 01 0.79503836E 00 0.21788097E-01-0.13456754E-04    3
-0.12698753E-09 0.25865213E-11 0.10379887E 05 0.18248696E 02                   4
N2O                 J12/64N   20    100   000   0G    300.000  5000.000        1
 0.47306679E 01 0.28258267E-02-0.11558115E-05 0.21263683E-09-0.14564087E-13    2
 0.81617682E 04-0.17151073E 01 0.26139195E 01 0.86439616E-02-0.68110624E-05    3
 0.22275577E-08-0.80650330E-13 0.87590123E 04 0.92266952E 01                   4
N2O4                J 9/64N   20    400   000   0G    300.000  5000.000        1
 0.10506637E 02 0.58723267E-02-0.24766296E-05 0.46556024E-09-0.32402082E-13    2
-0.28609096E 04-0.26252230E 02 0.36662865E 01 0.23491748E-01-0.16007297E-04    3
 0.11845939E-08 0.20001618E-11-0.90631797E 03 0.93973337E 01                   4
NA(S)               J 6/62NA  10    00    00    0S    300.000   370.980        1
 0.             0.             0.             0.             0.                2
 0.             0.             0.24118570E 01 0.89751859E-03 0.10583331E-04    3
-0.71915700E-08-0.55226618E-11-0.83575157E 03-0.82157280E 01                   4
NA(L)               J 6/62NA  10    00    00    0L    370.980  2000.000        1
 0.40097373E 01-0.12933184E-02 0.42443918E-06 0.52381272E-09-0.18396802E-12    2
-0.78115472E 03-0.15366128E 02 0.45673226E 01-0.25267108E-02 0.14840018E-05    3
 0.38590020E-10-0.82500845E-13-0.97421906E 03-0.18377804E 02                   4
NA                  J 6/62NA  100   000   000   0G    300.000  5000.000        1
 0.25623078E 01-0.13963284E-03 0.11292708E-06-0.42307732E-10 0.67057055E-14    2
 0.12193782E 05 0.38957727E 01 0.24881226E 01 0.85426102E-04-0.21514228E-06    3
 0.22671537E-09-0.85125266E-13 0.12215904E 05 0.42804839E 01                   4
NA+                 J 3/65NA  1E   -100   000   0G    300.000  5000.000        1
 0.25000000E 01 0.             0.             0.             0.                2
 0.72599320E 05 0.35374014E 01 0.25000000E 01 0.             0.                3
 0.             0.             0.72599330E 05 0.35374014E 01                   4
NACL                J12/64NA  1CL   100   000   0G    300.000  5000.000        1
 0.44282931E 01 0.15627241E-03-0.23103383E-07 0.47163571E-11-0.28832557E-15    2
-0.23170900E 05 0.22878194E 01 0.37032286E 01 0.31997608E-02-0.48924502E-05    3
 0.34639218E-08-0.91357521E-12-0.23028276E 05 0.57603243E 01                   4
NAF                 J 6/64NA  1F    100   000   0G    300.000  5000.000        1
 0.43344945E 01 0.25795040E-03-0.75672062E-07 0.14032381E-10-0.95933344E-15    2
-0.36623273E 05 0.12782548E 01 0.31808578E 01 0.44436924E-02-0.69860535E-05    3
 0.46184859E-08-0.11271357E-11-0.36384925E 05 0.68634707E 01                   4
NAH                 J 3/62NA  1H    100   000   0G    300.000  5000.000        1
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 0.38130579E 01 0.85643800E-03-0.31226816E-06 0.58502471E-10-0.40513924E-14    2
 0.13683062E 05 0.47100285E 00 0.31203350E 01 0.13996217E-02 0.27141234E-05    3
-0.39950795E-08 0.16726173E-11 0.13940065E 05 0.43813959E 01                   4
NAO                 J12/67NA  10   10   00   0G   300.000  5000.000            1
 0.43924158E 01 0.21320574E-03-0.45220543E-07 0.79751821E-11-0.51735989E-15    2
 0.87118995E 04 0.23749263E 01 0.34421007E 01 0.41617241E-02-0.63118368E-05    3
 0.44473194E-08-0.11720486E-11 0.89011477E 04 0.69371625E 01                   4
NAO-                J12/67NA  10   1E   10   0G   300.000  5000.000            1
 0.43368008E 01 0.22344672E-03-0.48212472E-07 0.85720862E-11-0.56094334E-15    2
-0.15946258E 05 0.10004509E 01 0.34186855E 01 0.42117382E-02-0.63164646E-05    3
 0.43873515E-08-0.11372639E-11-0.15752234E 05 0.56553725E 01                   4
NAOH(S)             J 3/66NA  10   1H   100  0S   300.000  592.250             1
 0.             0.             0.             0.             0.                2
 0.             0.             0.69758356E 01 0.13845689E-01-0.11496912E-03    3
 0.30593796E-06-0.22897632E-09-0.53448255E 05-0.33190509E 02                   4
NAOH(L)             J 3/66NA  10   1H   100  0L   592.250  5000.000            1
 0.10774143E 02-0.70452125E-03 0.             0.             0.                2
-0.53503303E 05-0.52256989E 02 0.10774143E 02-0.70452126E-03 0.                3
 0.             0.            -0.53503303E 05-0.52256989E 02                   4
NAOH                J 3/66NA  10   1H   100  0G   300.000  5000.000            1
 0.44705193E 01 0.19253365E-02-0.62522237E-06 0.95321167E-10-0.55722350E-14    2
-0.26808187E 05 0.23116081E 01 0.37588137E 01 0.41793587E-02-0.26908011E-05    3
 0.22226965E-09 0.39074039E-12-0.25645967E 05 0.59652624E 01                   4
NA2                 J 6/62NA  200  000  000  0G   300.000  5000.000            1
 0.44923659E 01 0.19571653E-03 0.22658417E-08-0.10132954E-11 0.13965752E-15    2
 0.15136031E 05 0.20044163E 01 0.43197514E 01 0.91397957E-03-0.11333878E-05    3
 0.79239225E-09-0.20379358E-12 0.15220419E 05 0.28326974E 01                   4
NA2CL2              J12/64NA  2CL  200  000  0G   300.000  5000.000            1
 0.98262001E 01 0.19184763E-03-0.81608743E-07 0.15298181E-10-0.10558994E-14    2
-0.71077149E 05-0.17049256E 02 0.79583953E 01 0.83962360E-02-0.13817116E-04    3
 0.10277666E-07-0.28544994E-11-0.70725939E 05-0.51334799E 01                   4
NA2F2               J 6/64NA  2F   200  000  0G   300.000  5000.000            1
 0.97228777E 01 0.30413632E-03-0.12867473E-06 0.24005001E-10-0.16439168E-14    2
-0.10137399E 06-0.19427619E 02 0.69101947E 01 0.12497812E-01-0.20283984E-04    3
 0.14892684E-07-0.40960013E-11-0.10134300E 06-0.60424822E 01                   4
NE                  L 5/66NE  100  000  000  0G   300.000  5000.000            1
 0.25000000E 01 0.             0.             0.             0.                2
-0.74537506E 03 0.33420436E 01 0.25000000E 01 0.             0.                3
 0.             0.            -0.74537498E 03 0.33420438E 01                   4
NE+                 L12/66NE  1E  -100  000  0G   300.000  5000.000            1
 0.29285147E 01-0.41229320E-03 0.16341709E-06-0.29554891E-10 0.20056917E-14    2
 0.25015219E 06 0.24159397E 01 0.21006406E 01 0.32416425E-02-0.56265881E-05    3
 0.38693679E-08-0.93291304E-12 0.25029535E 06 0.63098678E 01                   4
O                   J 6/62O   100  000  000  0G   300.000  5000.000            1
 0.25420594E 01-0.27550619E-04-0.31028033E-08 0.45510674E-11-0.43680515E-15    2
 0.29230803E 05 0.49203080E 01 0.29464287E 01-0.16381665E-02 0.24210316E-05    3
-0.16028432E-08 0.38906964E-12 0.29147644E 05 0.29639949E 01                   4
O+                  L12/66O   1E  -100  000  0G   300.000  5000.000            1
 0.25060488E 01-0.14464249E-04 0.12446049E-07-0.46958472E-11 0.65548873E-15    2
 0.18794765E 06 0.43479741E 01 0.24984794E 01 0.11410972E-04-0.29761395E-07    3
 0.32246539E-10-0.12375517E-13 0.18793408E 06 0.43864355E 01                   4
O-                  J 6/66O   1F   100  000  0G   300.000  5000.000            1
 0.25437173E 01-0.53252700E-04 0.25119617E-07-0.51351465E-11 0.39011542E-15    2
 0.11480516E 05 0.45202538E 01 0.29115796E 01-0.11975697E-02 0.18710553E-05    3
-0.13479179E-08 0.36663754E-12 0.11428431E 05 0.32402859E 01                   4
OH                  J 3/66O   1H   100  000  0G   300.000  5000.000            1
 0.29106427E 01 0.95931650E-03-0.19441702E-06 0.13756646E-10 0.14224542E-15    2
 0.39353815E 04 0.54423445E 01 0.38375943E 01-0.10778856E-02 0.96830378E-06    3
 0.18713972E-09-0.22571094E-12 0.35412823E 04 0.49370009E 00                   4
OH+                 J 3/66O   1H   1E  -100  0G   300.000  5000.000            1
 0.27544309E 01 0.15025381E-02-0.49411191E-06 0.79367805E-10-0.49153427E-14    2
 0.15759366E 06 0.60078407E 01 0.35447365E 01-0.19370343E-03-0.54786182E-06    3
 0.18897588E-08-0.94577482E-12 0.15736596E 06 0.13137392E 01                   4
OH-                 J 3/66O   1H   1F   100  0G   300.000  5000.000            1
 0.28772416E 01 0.99323674E-03-0.21102064E-06 0.17074239E-10-0.10219622E-15    2
-0.13124287E 05 0.42625863E 01 0.34554504E 01 0.45712434E-03-0.14994214E-05    3
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 0.19713519E-08-0.70807531E-12-0.14351948E 05 0.97534167E 00                   4
C2                   J 9/65O   20    00    00    0G    300.000  5000.000        1
 0.36219535E 01 0.73618264E-03-0.19652228E-06 0.36201558E-10-0.28945627E-14    2
-0.12019825E 04 0.36150960E 01 0.36255985E 01-0.18782184E-02 0.70554544E-05    3
-0.67635137E-08 0.21555993E-11-0.10475226E 04 0.43052778E 01                   4
O2-                  J12/66O   2E   100   000    0G    300.000  5000.000        1
 0.33147234E 01 0.77444546E-03-0.30677649E-06 0.56618118E-10-0.38229492E-14    2
-0.69913087E 04 0.29527995E 01 0.31440529E 01 0.12127972E-02 0.23812161E-05    3
-0.40914092E-08 0.16885304E-11-0.67369752E 04 0.67658687E 01                   4
P                    J 6/62P  100   000   000    0G    300.000  5000.000        1
 0.26307628E 01-0.17633559E-03 0.12025113E-07 0.33742455E-10-0.56423035E-14    2
 0.39352993E 05 0.46295137E 01 0.25016145E 01-0.71502000E-05 0.17900957E-07    3
-0.19050206E-10 0.73374466E-14 0.30407793E 05 0.53655588E 01                   4
P(S)                 J 6/61P   10    00    00    0S    300.000   900.000        1
 0.             0.             0.             0.             0.                2
 0.             0.             0.11869142E 01 0.75957720E-02-0.13635426E-04    3
 0.13366476E-07-0.47391960E-11-0.59485421E 03-0.57859428E 01                   4
P+                   L12/66P   1E  -100   000    0G    300.000  5000.000        1
 0.29021547E 01-0.58878893E-03 0.31298119E-06-0.59727539E-10 0.39304925E-14    2
 0.16204407E 06 0.38205693E 01 0.43790417E 01-0.64666723E-02 0.99340962E-05    3
-0.54858021E-08 0.12098857E-11 0.16174775E 06-0.33068769E 01                   4
PCL3                 J 9/62P  1CL   300   000    0G    300.000  5000.000        1
 0.94865575E 01 0.56885645E-03-0.24353840E-06 0.46003911E-10-0.32010959E-14    2
-0.33707085E 05-0.17113973E 02 0.53688177E 01 0.17665249E-01-0.27280124E-04    3
 0.19090652E-07-0.49399143E-11-0.32539165E 05 0.26507301E 01                   4
PF3                  J12/63P   1F   300   000    0G    300.000  5000.000        1
 0.84299114E 01 0.17487864E-02-0.75719927E-06 0.14491909E-09-0.10220929E-13    2
-0.10958235E 06-0.16492072E 02 0.23718086E 01 0.22753583E-01-0.27497236E-04    3
 0.14330466E-07-0.24023335E-11-0.10818123E 06 0.13590601E 02                   4
PH                   J 6/67P   1H   100   000    0G    300.000  5000.000        1
 0.30745442E 01 0.11698947E-02-0.30381654E-06 0.44436314E-10-0.27000975E-14    2
 0.29525775E 05 0.57548835E 01 0.36803433E 01-0.12756018E-02 0.25932442E-05    3
-0.84354107E-09-0.17208609E-12 0.29433909E 05 0.29054762E 01                   4
PH3                  J 6/62P   1H   300   000    0G    300.000  5000.000        1
 0.33448794E 01 0.65770941E-02-0.26336755E-05 0.47744660E-09-0.32354390E-13    2
 0.17337666E 04 0.39416278E 01 0.31581935E 01 0.24941492E-02 0.90255253E-05    3
-0.10227904E-07 0.32834250E-11 0.16387861E 04 0.62240564E 01                   4
PN                   J 9/62P   1N   100   000    0G    300.000  5000.000        1
 0.36419226E 01 0.94460672E-03-0.38923480E-06 0.73215826E-10-0.50961632E-14    2
 0.11333688E 05 0.41772775E 01 0.33755239E 01-0.41009386E-03 0.51265151E-05    3
-0.59473393E-08 0.21213592E-11 0.11578540E 05 0.60397418E 01                   4
PO                   J12/60P   1O   100   000    0G    300.000  5000.000        1
 0.38389008E 01 0.73137263E-03-0.29549285E-06 0.55085807E-10-0.33004882E-14    2
-0.19713892E 04 0.45600736E 01 0.39692758E 01-0.22016040E-02 0.77324127E-05    3
-0.78250095E-08 0.26509901E-11-0.18721788E 04 0.45414990E 01                   4
PS                   J 6/67P   1S   100   000    0G    300.000  5000.000        1
 0.43563526E 01 0.20240865E-03-0.78680674E-07 0.15193435E-10-0.81648513E-15    2
 0.93838309E 04 0.32161159E 01 0.37492824E 01 0.24320574E-02-0.31[illegible]E-05    3
 0.17650760E-08-0.34202790E-12 0.95171437E 04 0.61975908E 01                   4
P2                   J 6/61P  200   000   000    0G    300.000  5000.000        1
 0.41611733E 01 0.39620809E-03-0.15580339E-06 0.29093474E-10-0.20042459E-14    2
 0.20148756E 05 0.22279293E 01 0.23391107E 01 0.48266193E-02-0.54947488E-05    3
 0.25808507E-08-0.32236453E-12 0.20459594E 05 0.83232470E 01                   4
P4                   J 6/61P  400   000   000    0G    300.000  5000.000        1
 0.92252739E 01 0.36894123E-03-0.37758338E-06 0.72379666E-10-0.51066109E-14    2
 0.12490323E 05-0.19654868E 02 0.35353390E 01 0.24125292E-01-0.36462759E-04    3
 0.24916906E-07-0.63298563E-11 0.13635307E 05 0.77427326E 01                   4
S(S)                 J12/65S   10    00    00    0S    300.000   388.360        1
 0.             0.             0.             0.             0.                2
 0.             0.            -0.50637425E 01 0.28319353E-02-0.21330205E-04    3
 0.84737862E-06-0.17344967E-08 0.71487629E 03 0.28714074E 02                   4
S(L)                 J12/65S   10    00    00    0L    388.360  2000.000        1
 0.36536672E 01 0.99033405E-03-0.10114410E-05 0.40536327E-09-0.56679135E-13    2
-0.84538383E 03-0.16344703E 02-0.12063108E 02 0.90725716E-01-0.16951796E-03    3
 0.13070237E-06-0.35276150E-10 0.12346069E 04 0.55210160E 02                   4
S                    J12/65S  100   000   000    0G    300.000  5000.000        1
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 0.29119165E 01-0.56050635E-03 0.23155555E-06-0.50994912E-10 0.31945420E-14    2
 0.32726267E 05 0.37725044E 01 0.29293157E 01 0.19994093E-03-0.23314920E-05    3
 0.28521102E-08-0.10656090E-11 0.32686945E 05 0.35000372E 01                   4
S+               L12/66S   1E  -100  000  0G   300.000  5000.000               1
 0.24118653E 01 0.22103303E-03-0.18939564E-06 0.61336675E-10-0.53887720E-14    2
 0.15375732E 06 0.58861130E 01 0.25038214E 01-0.62475561E-04 0.15513305E-06    3
-0.16148749E-09 0.60012103E-13 0.15373003E 06 0.53857186E 01                   4
SF4              J 9/65S   1F   400  000  0G   300.000  5000.000               1
 0.10753578E 02 0.25135146E-02-0.10920195E-05 0.20962472E-09-0.14820130E-13    2
-0.91407009E 05-0.28295056E 02 0.65243888E 00 0.39223804E-01-0.50882839E-04    3
 0.29292955E-07-0.59164774E-11-0.89149574E 05 0.21447238E 02                   4
SF6              J 9/65S   1F   600  000  0G   300.000  5000.000               1
 0.15286816E 02 0.41541264E-02-0.18053249E-05 0.34670689E-09-0.24523633E-13    2
-0.15234672E 06-0.55069672E 02-0.11646703E 01 0.64060912E-01-0.83337512E-04    3
 0.48244600E-07-0.98455246E-11-0.14868151E 06 0.25921767E 02                   4
SH               J 6/67S   1H   100  000  0G   300.000  5000.000               1
 0.30371352E 01 0.12752466E-02-0.42314345E-06 0.67719668E-10-0.40934312E-14    2
 0.16545437E 05 0.60722981E 01 0.44098953E 01-0.22063747E-02 0.13171081E-05    3
 0.16467179E-08-0.12144787E-11 0.16180734E 05-0.10226129E 01                   4
SN               J 6/61S   1N   100  000  0G   300.000  5000.000               1
 0.38493376E 01 0.72756788E-03-0.29370203E-06 0.55013628E-10-0.38123551E-14    2
 0.30459962E 05 0.44179139E 01 0.39422971E 01-0.20035515E-02 0.73534644E-05    3
-0.75168560E-08 0.25591098E-11 0.30563949E 05 0.45699484E 01                   4
SO               J12/65S   1O   100  000  0G   300.000  5000.000               1
 0.38280162E 01 0.75593144E-03-0.30791631E-06 0.57880156E-10-0.40204449E-14    2
-0.43632695E 03 0.44528198E 01 0.31224222E 01 0.13797342E-02 0.20611837E-05    3
-0.39700344E-08 0.16366249E-11-0.17547567E 03 0.84176931E 01                   4
SOF2             J 9/65S   1O   1F   200  0G   300.000  5000.000               1
 0.81678130E 01 0.20156607E-02-0.86557421E-06 0.16471939E-09-0.11566374E-13    2
-0.70763942E 05-0.14145544E 02 0.26905686E 01 0.20314017E-01-0.23187553E-04    3
 0.11328486E-07-0.16744583E-11-0.69453573E 05 0.13247064E 02                   4
SO2              J 6/61S   1O   200  000  0G   300.000  5000.000               1
 0.52451364E 01 0.19704204E-02-0.80375769E-06 0.15149969E-09-0.10558004E-13    2
-0.37558227E 05-0.10873524E 01 0.32665338E 01 0.53237902E-02 0.68437552E-06    3
-0.52810047E-08 0.25590454E-11-0.36905148E 05 0.96513476E 01                   4
SO2F2            J 3/63S   1O   2F   200  0G   300.000  5000.000               1
 0.97589416E 01 0.35349972E-02-0.15103050E-05 0.28648297E-09-0.20072393E-13    2
-0.10668096E 06-0.23029863E 02 0.26823217E 01 0.25219882E-01-0.24789168E-04    3
 0.93820305E-08-0.44501989E-12-0.10487605E 06 0.12832633E 02                   4
SO3              J 9/65S   1O   300  000  0G   300.000  5000.000               1
 0.70757376E 01 0.31763387E-02-0.13535760E-05 0.25630912E-09-0.17936044E-13    2
-0.50211376E 05-0.11200793E 02 0.25780385E 01 0.14556335E-01-0.91764173E-05    3
-0.79203022E-09 0.19709473E-11-0.48931753E 05 0.12251863E 02                   4
S2               J12/65S   200  000  000  0G   300.000  5000.000               1
 0.42051134E 01 0.35309150E-03-0.13543069E-06 0.25245375E-10-0.17357439E-14    2
 0.14182908E 05 0.32094717E 01 0.28724248E 01 0.50434461E-02-0.62055277E-05    3
 0.33097022E-08-0.57376103E-12 0.14487076E 05 0.93082405E 01                   4
SI(S)            J 3/67SI  100  000  000  0S   300.000  1685.000               1
 0.24753989E 01 0.38112187E-03-0.20939481E-06 0.42757187E-11 0.15006567E-13    2
-0.81255620E 03-0.12188747E 02 0.84197538E 00 0.63710416E-02-0.13077030E-04    3
 0.97593603E-08-0.27279380E-11-0.52486268E 03-0.45272678E 01                   4
SI(L)            J 3/67SI  100  000  000  0L  1685.000  5000.000               1
 0.32799915E 01 0.             0.             0.             0.                2
 0.48546547E 04-0.13289281E 02 0.             0.             0.                3
 0.             0.             0.             0.                               4
SI               J 3/67SI  100  000  000  0G   300.000  5000.000               1
 0.26506014E 01-0.35763852E-03 0.29592293E-06-0.72804829E-10 0.57963329E-14    2
 0.53437054E 05 0.52204057E 01 0.31793537E 01-0.27646992E-02 0.44784033E-05    3
-0.32833177E-08 0.91213631E-12 0.53339032E 05 0.27273204E 01                   4
SI+              L12/66SI  1E  -100  000  0G   300.000  5000.000               1
 0.26645138E 01-0.19505635E-03 0.39017068E-07-0.17361091E-10 0.13133569E-14    2
 0.14791314E 06 0.45229974E 01 0.30497015E 01-0.53831622E-02 0.70533565E-05    3
-0.52417458E-08 0.12637267E-11 0.14765904E 06-0.15631487E 01                   4
SIC              J 3/67ST  1C   100  000  0G   300.000  5000.000               1
 0.55799533E 01-0.13409344E-02 0.75483047E-06-0.16543778E-09 0.12663345E-13    2
 0.55946170E 05-0.56633593E 01-0.21924695E 01 0.41342700E-01-0.73274113E-04    3
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 0.60694120E-07-0.16729207E-10 0.85953143E 05 0.28756080E 02                   4
SIC2                  J 3/67SI  1C   200  000  0G   300.000  5000.000          1
 0.57011523E 01 0.21220690E-02-0.11457769E-05 0.31038768E-09-0.27763897E-13    2
 0.72023391E 05-0.49868951E 01 0.38816333E 01 0.67947767E-02-0.50277962E-05    3
 0.10573232E-08 0.25513142E-12 0.72558249E 05 0.45374042E 01                   4
SICL                  J 9/67SI  1CL  100  000  0G   300.000  5000.000          1
 0.44179424E 01 0.13137080E-03-0.30789013E-07 0.47802942E-11-0.24135145E-15    2
 0.21650362E 05 0.33226343E 01 0.33247525E 01 0.24980130E-02-0.36640266E-05    3
 0.25169051E-08-0.65148061E-12 0.21774076E 05 0.61967573E 01                   4
SICL2                 J12/60SI  1CL  200  000  0G   300.000  5000.000          1
 0.66401140E 01 0.40061524E-03-0.17252517E-06 0.32791504E-10-0.22955397E-14    2
-0.21042974E 05-0.44453305E 01 0.40946591E 01 0.10677550E-01-0.15924644E-04    3
 0.10778153E-07-0.26810463E-11-0.20524636E 05 0.73395733E 01                   4
SICL4                 J 9/67SI  1CL  400  000  0G   300.000  5000.000          1
 0.12083655E 02 0.10190735E-02-0.44167865E-06 0.84431573E-10-0.59491580E-14    2
-0.82936052E 05-0.29940036E 02 0.61040010E 01 0.24933114E-01-0.36703263E-04    3
 0.24448748E-07-0.60370155E-11-0.81705075E 05-0.98955289E 00                   4
SIF                   J12/63SI  1F   100  000  0G   300.000  5000.000          1
 0.41464751E 01 0.42486929E-03-0.15054738E-06 0.29852749E-10-0.20491743E-14    2
-0.18225468E 04 0.32442007E 01 0.33165872E 01 0.24504639E-02-0.11611721E-05    3
-0.84034933E-09 0.67357144E-12-0.15893631E 04 0.75729103E 01                   4
SIF2                  J 6/68SI  1F   20   00   0G   300.000  5000.000          1
 0.60363216E 01 0.11224411E-02-0.51297359E-06 0.10224952E-09-0.68931139E-14    2
-0.75992284E 05-0.42683330E 01 0.29399908E 01 0.11414220E-01-0.12738714E-04    3
 0.57841411E-08-0.65849149E-12-0.75256749E 05 0.11210391E 02                   4
SIF4                  J 9/63SI  1F   400  000  0G   300.000  5000.000          1
 0.10545038E 02 0.27200200E-02-0.11741279E-05 0.22433362E-09-0.15803156E-13    2
-0.13792290E 06-0.27951944E 02 0.31059749E 01 0.26866992E-01-0.29186297E-04    3
 0.12874579E-07-0.13517263E-11-0.19611327E 06 0.94141918E 01                   4
SIH                   J12/60SI  1H   100  000  0G   300.000  5000.000          1
 0.30623551E 01 0.14953654E-02-0.56220832E-06 0.10102854E-09-0.67870459E-14    2
 0.56371778E 05 0.59817282E 01 0.37346289E 01-0.19725978E-02 0.51154518E-05    3
-0.35400381E-08 0.75850849E-12 0.56301206E 05 0.23754228E 01                   4
SIH4                  J12/60SI  1H   400  000  0G   300.000  5000.000          1
 0.44433856E 01 0.86334212E-02-0.35060000E-05 0.64194983E-09-0.43824526E-13    2
 0.13468284E 04-0.40777748E 01 0.17519579E 01 0.11564482E-01 0.10586376E-05    3
-0.75058684E-08 0.31897221E-11 0.28880916E 04 0.11103122E 02                   4
SIN                   J 3/67SI  1N   100  000  0G   300.000  5000.000          1
 0.39858621E 01-0.87927056E-05 0.54269539E-06-0.17951017E-09 0.16337069E-13    2
 0.43524809E 05 0.31615156E 01 0.31051955E 01 0.14352449E-02 0.18561060E-05    3
-0.37734383E-08 0.16835331E-11 0.43785703E 05 0.78753961E 01                   4
SIO                   J 9/67SI  1O   100  000  0G   300.000  5000.000          1
 0.37473335E 01 0.81991943E-03-0.32525396E-06 0.57324962E-10-0.35108944E-14    2
-0.13317430E 05 0.36478404E 01 0.32528276E 01 0.41823126E-03 0.37806202E-05    3
-0.51024483E-08 0.19471317E-11-0.13090340E 05 0.66485803E 01                   4
SIO2(S)               J 6/67SI  1O   200  000  0S   300.000   847.000          1
 0.             0.             0.             0.             0.                2
 0.             0.             0.37282163E 00 0.21562223E-01-0.14573894E-04    3
-0.83303379E-08 0.12526015E-10-0.11048161E 06-0.28621543E 01                   4
SIO2(S)               J 6/67SI  1O   200  000  0S   847.000  1079.000          1
 0.70854710E 01 0.12077507E-02 0.             0.             0.                2
-0.11178740E 06-0.36198180E 02 0.70854710E 01 0.12077507E-02 0.                3
 0.             0.            -0.11178740E 06-0.36198180E 02                   4
SIO2(S)               J 6/67SI  1O   200  000  0S  1079.000  1996.000          1
 0.66032335E 01 0.25956500E-02-0.69075293E-06-0.17550104E-09 0.82131540E-13    2
-0.11150871E 06-0.33656253E 02 0.             0.             0.                3
 0.             0.             0.             0.                               4
SIO2(L)               J 6/67SI  1O   200  000  0L  1996.000  5000.000          1
 0.10316204E 02 0.             0.             0.             0.                2
-0.11460598E 06-0.57629533E 02 0.             0.             0.                3
 0.             0.             0.             0.                               4
SIC2                  J 9/67SI  1C   200  000  0G   300.000  5000.000          1
 0.53620395E 01 0.17719734E-02-0.75194104E-06 0.14180584E-09-0.98856417E-14    2
-0.38767316E 05-0.68603501E 01 0.37628058E 01 0.85016594E-02-0.57388144E-05    3
 0.12896573E-10 0.97544976E-12-0.38035971E 05 0.65549123E 01                   4
SIS                   J12/60SI  1S   100  000  0G   300.000  5000.000          1
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 0.41729993E 01 0.39458404E-03-0.16004302E-06 0.30841978E-10-0.21886645E-14    2
 0.71535070E 04 0.25342404E 01 0.25507345E 01 0.49535017E-02-0.59703409E-05    3
 0.30600985E-08-0.45754490E-12 0.74929393E 04 0.93959024E 01                   4
SI2                J 3/67SI  200  000  000  0G   300.000  5000.000             1
 0.50474139E-01 0.53990034E-03-0.43078376E-06 0.11355206E-09-0.96262871F-14    2
 0.69133185E 05-0.19234578E 01 0.38155393E 01-0.19096547E-03 0.59233416E-05    3
-0.57649503E-08 0.14775004E-11 0.69784655E 05 0.57275556E 01                   4
SI2C               J 3/67SI  2C   100  000  0G   300.000  5000.000             1
 0.62510388E 01 0.13224176F-02-0.72605214E-06 0.23269424F-09-0.23285148E-13    2
 0.62300999E 05-0.72966415E 01 0.40433933E 01 0.73456957E-02-0.66412549E-05    3
 0.24885047E-08-0.18196555E-12 0.62935417E 05 0.41712491E 01                   4
SI2N               J 3/67SI  2N   100  000  0G   300.000  5000.000             1
 0.66709912E 01 0.91917882E-03-0.39517130E-06 0.74397145E-10-0.50284691E-14    2
 0.45620154E 05-0.78114415E 01 0.36686735E 01 0.11301840E-01-0.13637119E-04    3
 0.71653050E-08-0.12378310E-11 0.46313033E 05 0.71095459E 01                   4
SI3                J 3/67SI  300  000  000  0G   300.000  5000.000             1
 0.74213360E 01-0.11703943E-03 0.89820775E-07 0.71935964E-11-0.25670837E-14    2
 0.74146699E 05-0.10365274E 02 0.45979129E 01 0.10715274F-01-0.16100422E-04    3
 0.10969207E-07-0.27832875E-11 0.74766324E 05 0.34421671E 01                   4
END           LAST CARC
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